

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
 Data File : BM046359.D
 Acq On : 28 Jun 2024 19:23
 Operator : MA/JU
 Sample : P3115-12 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VNJ-325

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.593	281	290	306	rVB	121503	292738	1.87%	0.121%
2	5.051	361	368	387	rBV	1292147	2312979	14.76%	0.955%
3	6.628	630	636	647	rBV	1209856	2244990	14.33%	0.927%
4	7.375	757	763	772	rVB	671898	1091145	6.96%	0.451%
5	7.904	848	853	860	rBV2	188904	320280	2.04%	0.132%
6	8.439	938	944	949	rBV	302709	485199	3.10%	0.200%
7	8.534	954	960	975	rVV	832259	1668610	10.65%	0.689%
8	8.863	1007	1016	1021	rBV	245345	470832	3.00%	0.194%
9	9.045	1040	1047	1056	rVB2	144057	325086	2.07%	0.134%
10	9.151	1056	1065	1073	rBV4	65104	201077	1.28%	0.083%
11	9.686	1151	1156	1166	rVV	478309	727852	4.64%	0.301%
12	9.786	1167	1173	1183	rVB2	194301	454445	2.90%	0.188%
13	10.128	1224	1231	1236	rBV	859163	1489453	9.50%	0.615%
14	10.181	1236	1240	1245	rVV	145904	274150	1.75%	0.113%
15	10.245	1246	1251	1257	rVV3	169377	334264	2.13%	0.138%
16	10.345	1257	1268	1276	rVB2	241026	582225	3.72%	0.240%
17	10.510	1287	1296	1301	rBV7	99072	243887	1.56%	0.101%
18	11.039	1378	1386	1390	rVB3	130403	314544	2.01%	0.130%
19	11.139	1399	1403	1407	rBV	222441	334363	2.13%	0.138%
20	11.357	1434	1440	1444	rBV	1281094	1956277	12.48%	0.808%
21	11.392	1444	1446	1451	rVB2	209493	264827	1.69%	0.109%
22	11.445	1452	1455	1458	rBV	137436	215444	1.37%	0.089%
23	11.545	1468	1472	1474	rBV2	208575	307740	1.96%	0.127%
24	11.722	1498	1502	1506	rBV2	443235	709530	4.53%	0.293%
25	11.827	1517	1520	1523	rBV4	150869	233486	1.49%	0.096%
26	11.916	1532	1535	1539	rVB	421600	527213	3.36%	0.218%
27	12.016	1549	1552	1554	rBV	235405	289368	1.85%	0.119%
28	12.098	1563	1566	1567	rBV2	206490	225973	1.44%	0.093%
29	12.310	1595	1602	1605	rBV3	840142	2010849	12.83%	0.830%
30	12.351	1606	1609	1612	rVB	939052	1182906	7.55%	0.488%
31	12.404	1612	1618	1623	rBV	3602315	5677061	36.23%	2.344%
32	12.510	1629	1636	1641	rBV2	1764914	4023071	25.67%	1.661%
33	12.569	1641	1646	1651	rVB	2775067	4517192	28.83%	1.865%
34	12.627	1651	1656	1665	rBV3	2380354	5779452	36.88%	2.387%
35	12.739	1670	1675	1677	rBV	1702211	2683714	17.13%	1.108%
36	12.951	1708	1711	1714	rVB	901453	988439	6.31%	0.408%

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
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37	13.057	1721	1729	1735	rVB	6524829	12359674	78.87%	5.104%
38	13.151	1742	1745	1749	rVB2	1481509	1831452	11.69%	0.756%
39	13.263	1761	1764	1767	rBV2	892680	1100636	7.02%	0.454%
40	13.327	1768	1775	1780	rBV3	1740473	4643925	29.63%	1.918%
41	13.474	1797	1800	1803	rBV3	1084314	1634739	10.43%	0.675%
42	13.739	1841	1845	1849	rBV2	2186411	3160957	20.17%	1.305%
43	13.827	1857	1860	1865	rVB2	2341140	3147135	20.08%	1.300%
44	13.969	1880	1884	1888	rBV	8113001	11768515	75.10%	4.860%
45	14.051	1896	1898	1902	rVB	1970104	2101913	13.41%	0.868%
46	14.804	2023	2026	2031	rBV2	3138290	4387822	28.00%	1.812%
47	14.974	2052	2055	2067	rVB	5146106	10530413	67.20%	4.348%
48	20.115	2925	2929	2935	rVB	6311230	9249584	59.02%	3.819%
49	20.315	2960	2963	2966	rVB	2636500	2903831	18.53%	1.199%
50	20.368	2968	2972	2975	rVV	6752983	8779272	56.02%	3.625%
51	20.427	2979	2982	2987	rVB	3177207	3905079	24.92%	1.613%
52	20.809	3043	3047	3053	rVB	7703939	9650651	61.58%	3.985%
53	20.874	3054	3058	3061	rBV	3512362	4363814	27.85%	1.802%
54	20.992	3074	3078	3082	rBV2	6168700	9964620	63.59%	4.115%
55	21.044	3085	3087	3093	rVB	5618800	6937043	44.27%	2.865%
56	21.268	3121	3125	3132	rVB	4986285	6745049	43.04%	2.785%
57	21.774	3207	3211	3217	rVB	4064287	5837097	37.25%	2.410%
58	22.056	3255	3259	3264	rVB	4159074	5802359	37.03%	2.396%
59	22.662	3356	3362	3369	rBV	3480300	6537564	41.72%	2.700%
60	22.868	3387	3397	3401	rBV	5467218	15671043	100.00%	6.471%
61	23.062	3425	3430	3436	rVB	703188	1350307	8.62%	0.558%
62	23.315	3468	3473	3482	rVB	2207368	4556818	29.08%	1.882%
63	23.450	3489	3496	3508	rVB	3395255	8183079	52.22%	3.379%
64	23.562	3508	3515	3524	rVB	3364103	7091911	45.25%	2.928%
65	23.738	3541	3545	3558	rVB3	977840	2987851	19.07%	1.234%
66	24.115	3603	3609	3618	rVB	1871832	4083581	26.06%	1.686%
67	24.550	3678	3683	3692	rVB	2086025	5071536	32.36%	2.094%
68	25.568	3849	3856	3865	rVB	1424225	3971602	25.34%	1.640%
69	26.638	4031	4038	4042	rBV2	939147	2595085	16.56%	1.072%
70	28.103	4280	4287	4302	rVB	900417	3505320	22.37%	1.447%

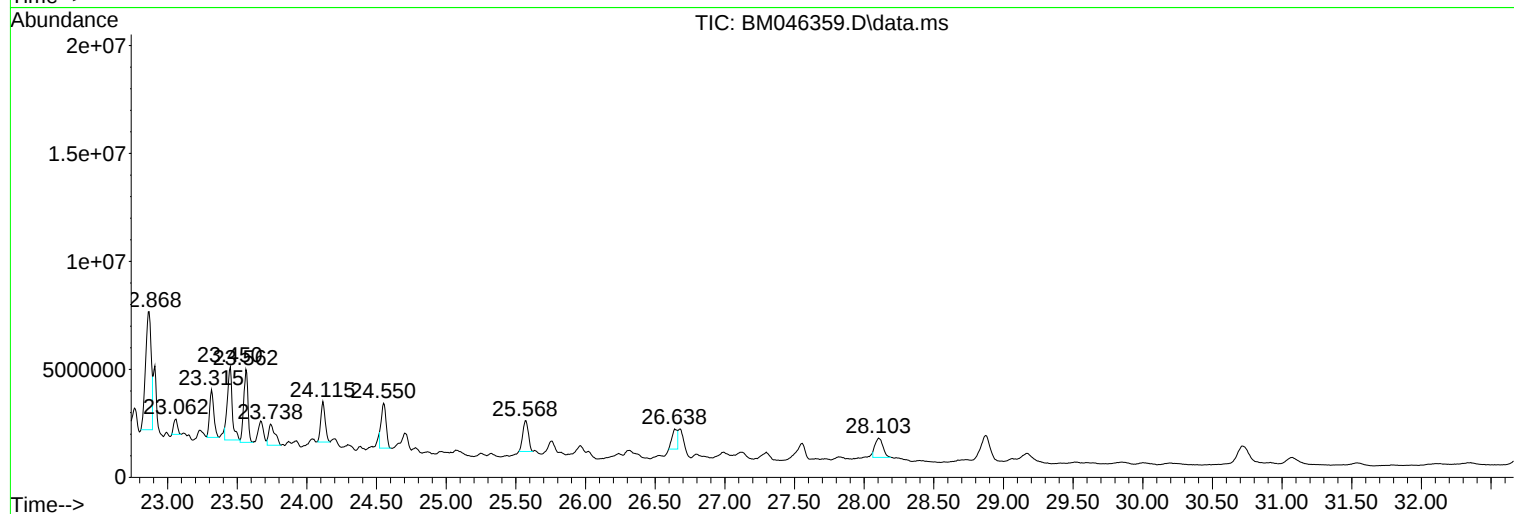
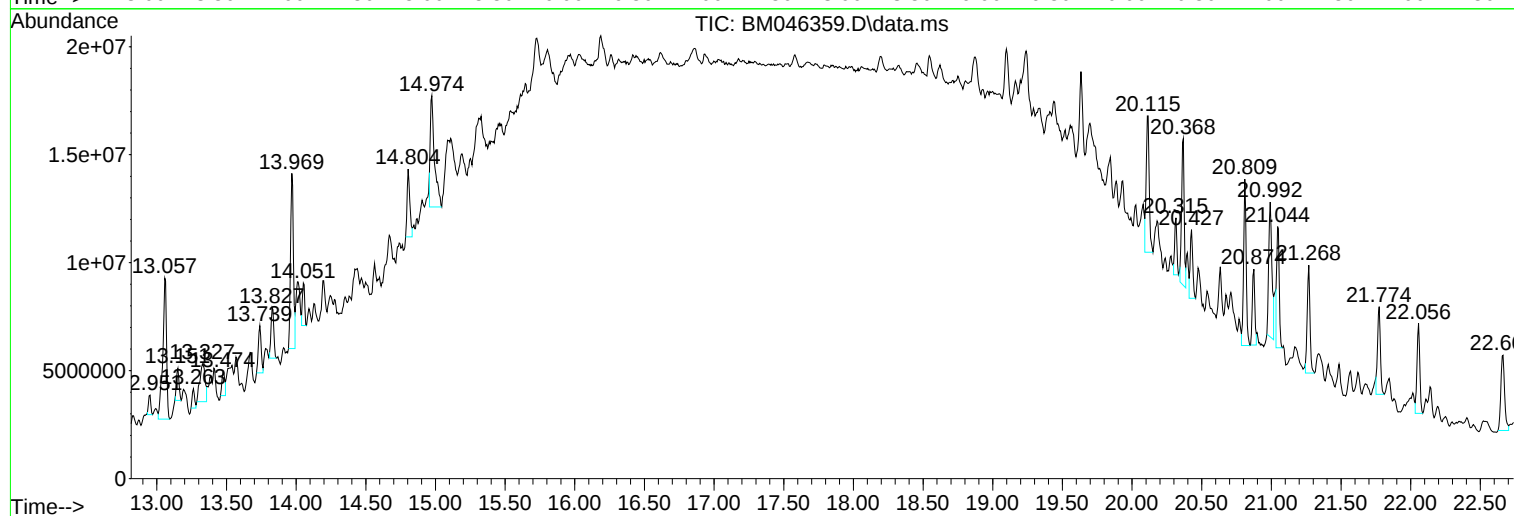
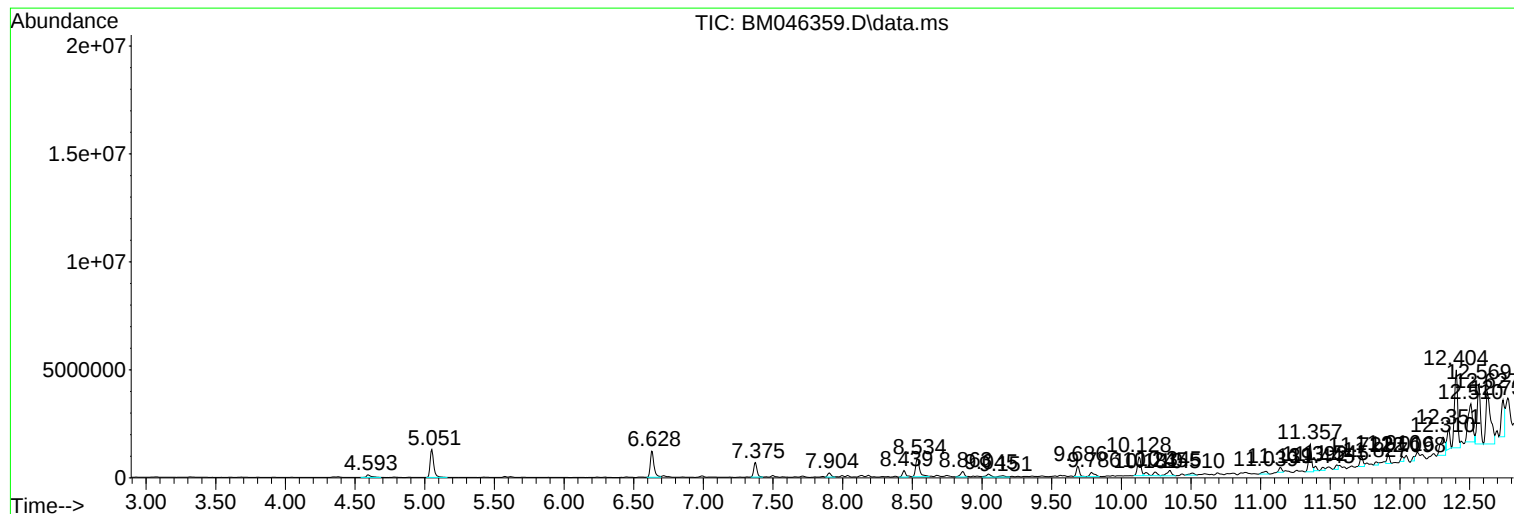
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Instrument :
BNA_M
ClientSampleId :
VNJ-325

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

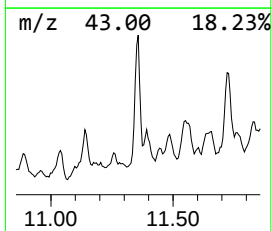
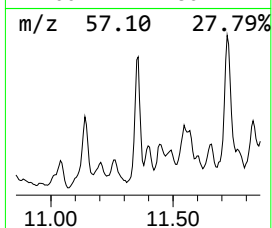
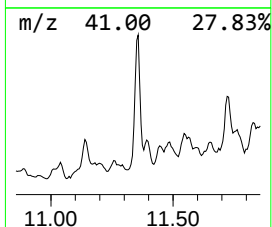
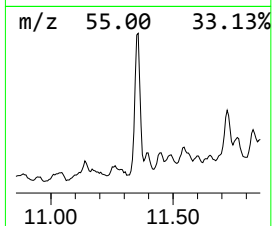
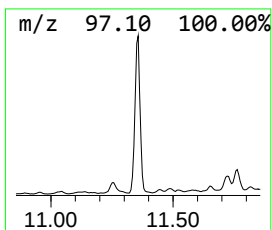
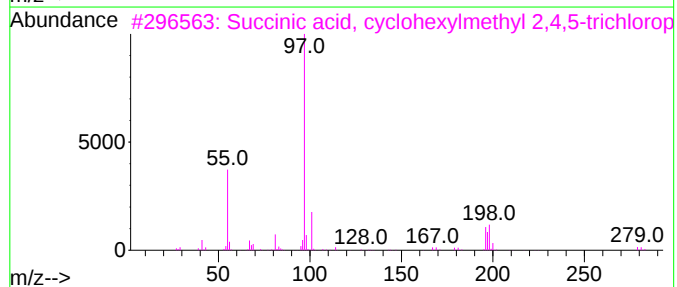
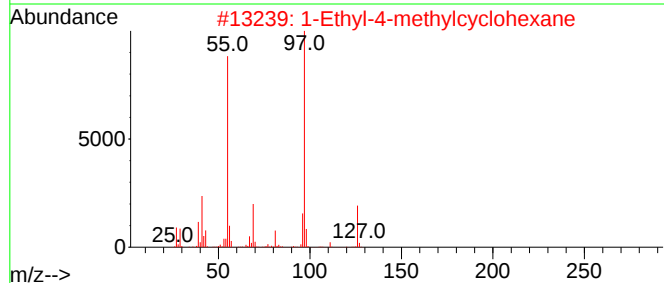
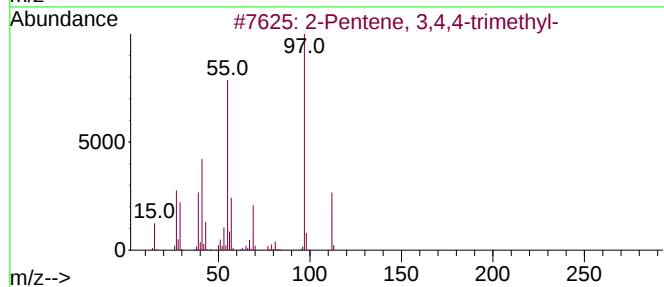
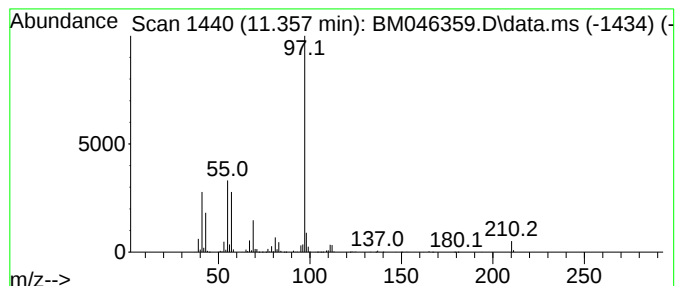
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentene, 3,4,4-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.357	26.27 ng	1956280	Naphthalene-d8	10.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4,4-trimethyl-			112	C8H16	000598-96-9	64
2	1-Ethyl-4-methylcyclohexane			126	C9H18	003728-56-1	64
3	Succinic acid, cyclohexylmethyl ...			392	C17H19Cl3O4	1000389-96-9	64
4	4-Hepten-3-one, 2,6-dimethyl-			140	C9H16O	056259-14-4	59
5	1-(Trimethylsilyl)-1-propyne			112	C6H12Si	006224-91-5	56



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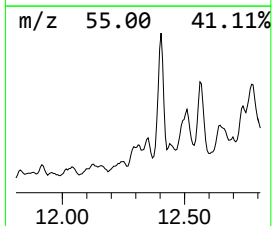
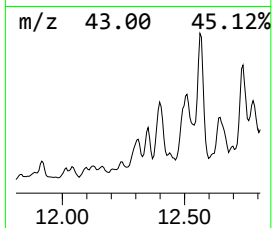
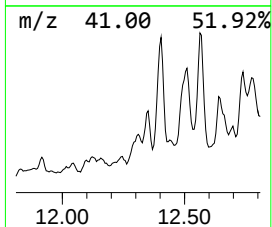
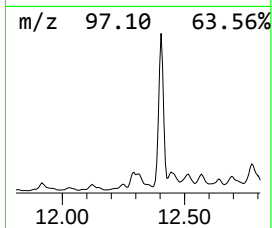
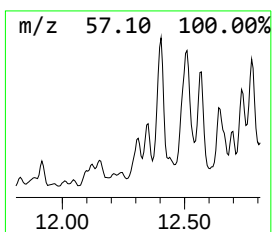
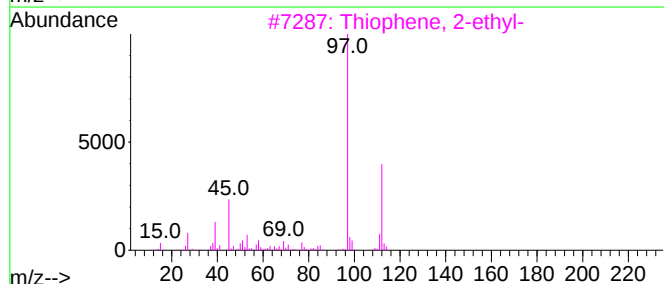
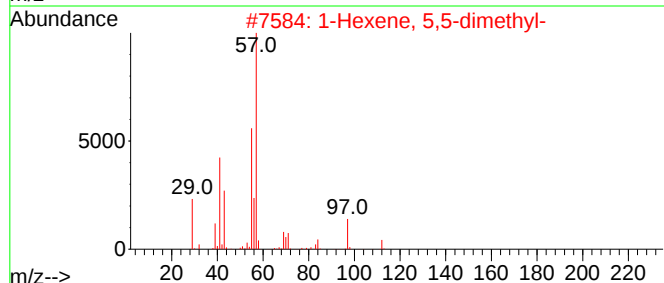
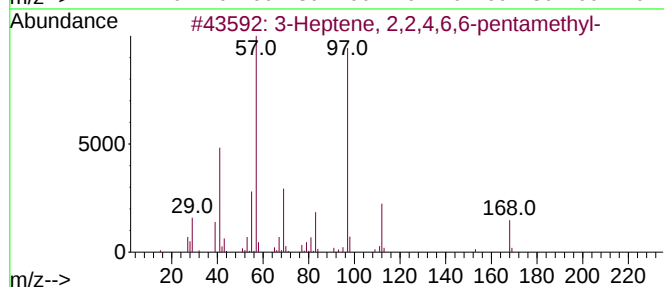
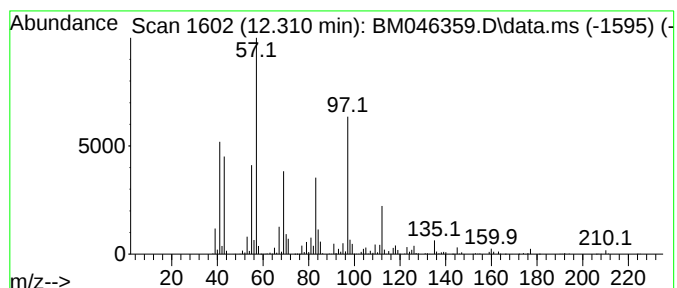
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Heptene, 2,2,4,6,6-pentam... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.310	19.13 ng	2010850	Acenaphthene-d10			14.015
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Heptene, 2,2,4,6,6-pentamethyl-		168	C12H24	000123-48-8	53
2	1-Hexene, 5,5-dimethyl-		112	C8H16	007116-86-1	50
3	Thiophene, 2-ethyl-		112	C6H8S	000872-55-9	43
4	Thiophene, 3-ethyl-		112	C6H8S	001795-01-3	43
5	Cyclohexane, 1,3-dimethyl-, trans-		112	C8H16	002207-03-6	43



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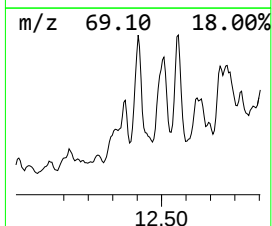
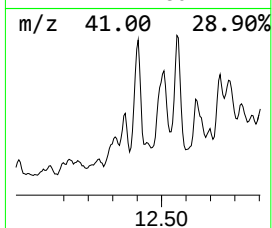
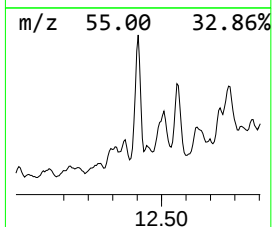
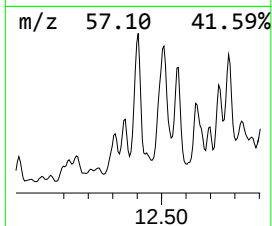
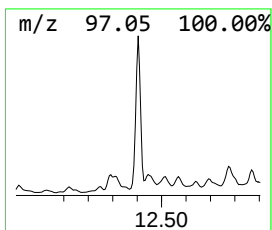
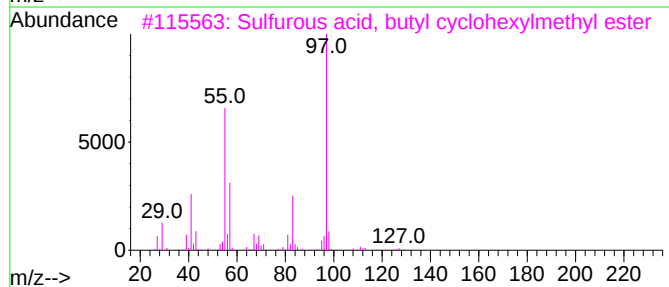
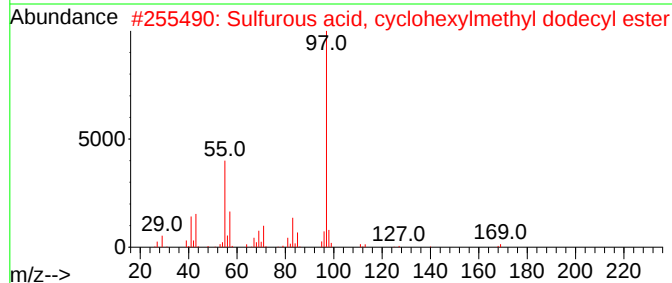
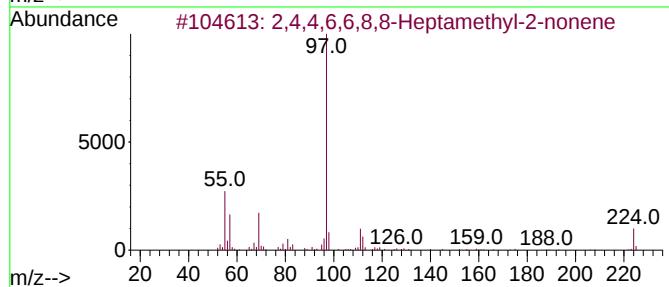
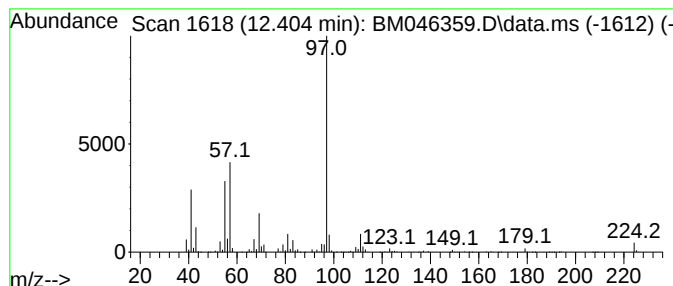
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.404	54.02 ng	5677060	Acenaphthene-d10	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	72
2	Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	64
3	Sulfurous acid, butyl cyclohexyl...	234	C11H22O3S	1000309-21-4	64
4	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64
5	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	64



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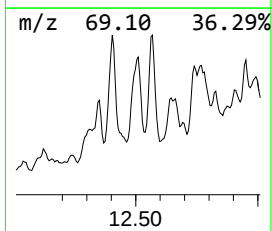
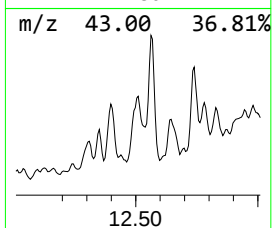
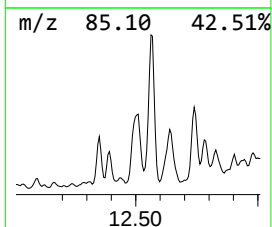
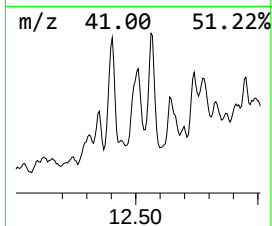
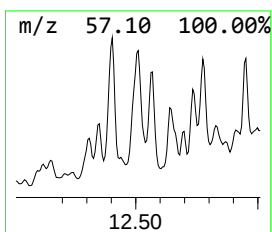
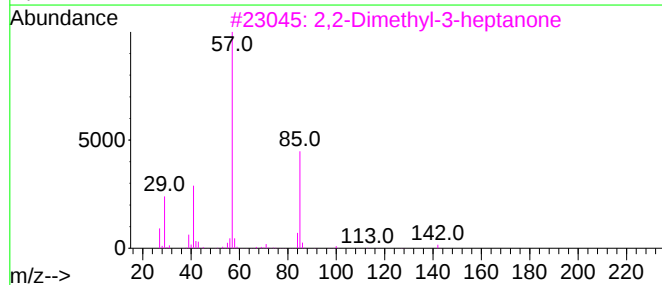
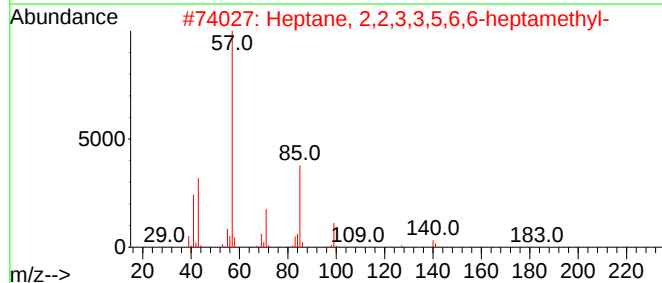
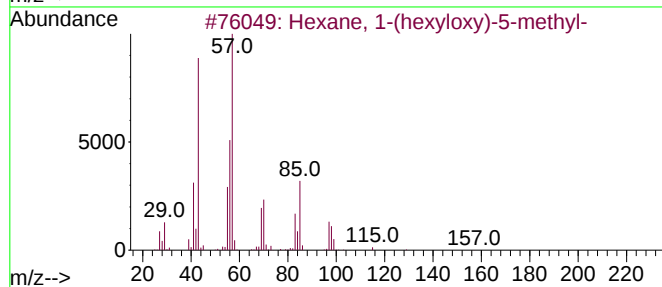
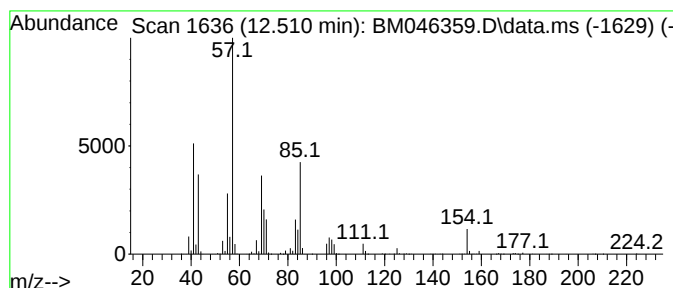
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ClientSampleId :
VNJ-325

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexane, 1-(hexyloxy)-5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.510	38.28 ng	4023070	Acenaphthene-d10	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	50
2	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	43
3	2,2-Dimethyl-3-heptanone	142	C9H18O	019078-97-8	43
4	4-Undecene, (Z)-	154	C11H22	000821-98-7	41
5	Decane, 3-ethyl-3-methyl-	184	C13H28	017312-66-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-325

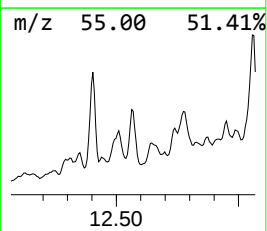
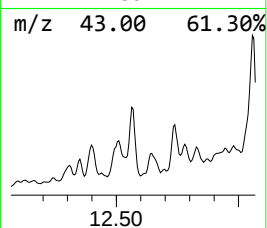
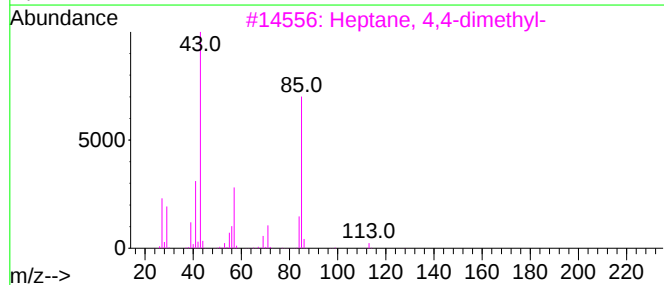
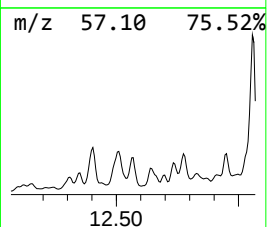
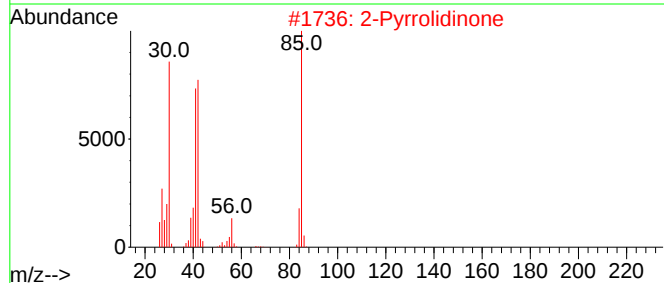
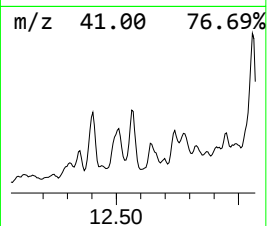
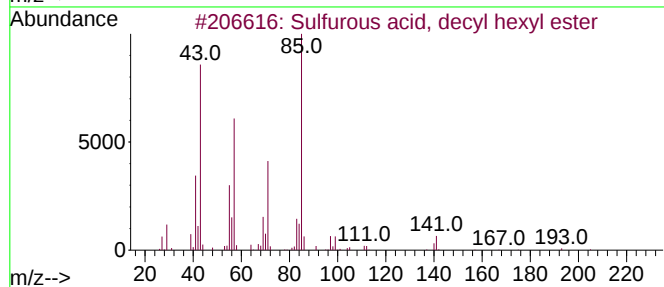
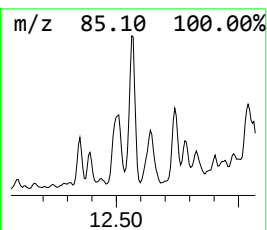
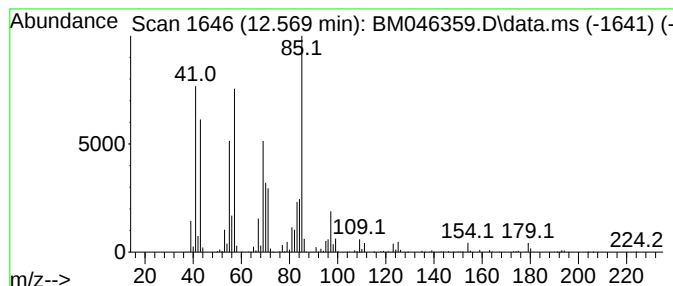
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, decyl hexyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	42.98 ng	4517190	Acenaphthene-d10	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl hexyl ester	306	C16H34O3S	1000309-13-2	50
2			2-Pyrrolidinone	85	C4H7NO	000616-45-5	43
3			Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	43
4			Pentane, 3-(bromomethyl)-	164	C6H13Br	003814-34-4	38
5			10-Methylundecan-4-olide	198	C12H22O2	1000370-40-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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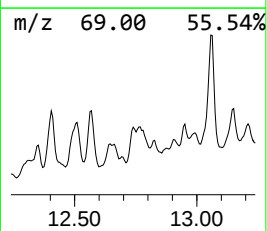
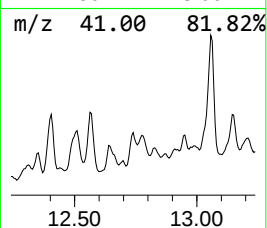
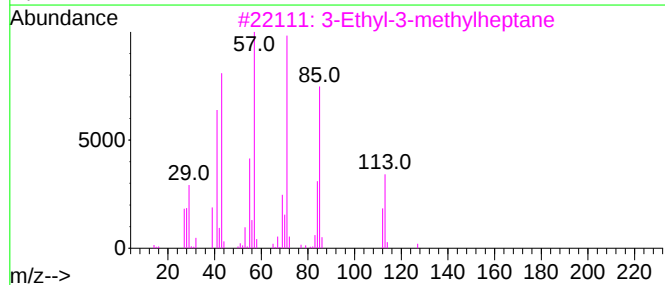
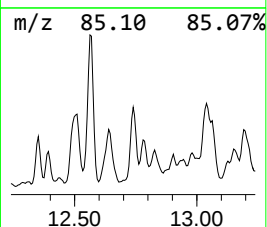
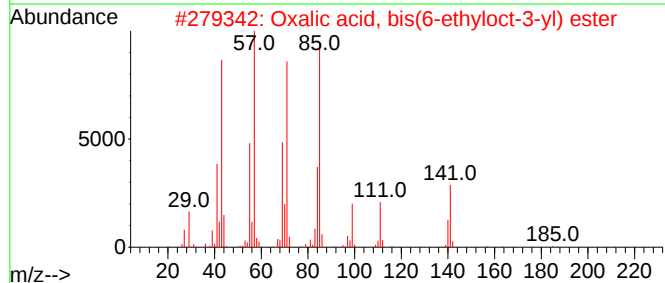
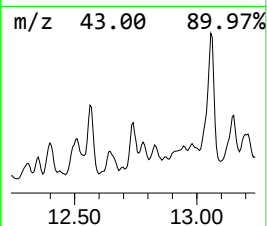
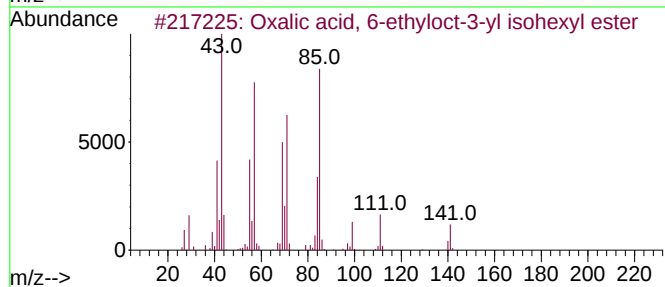
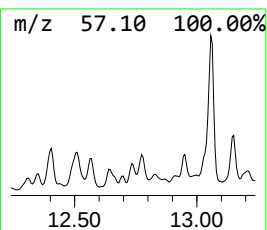
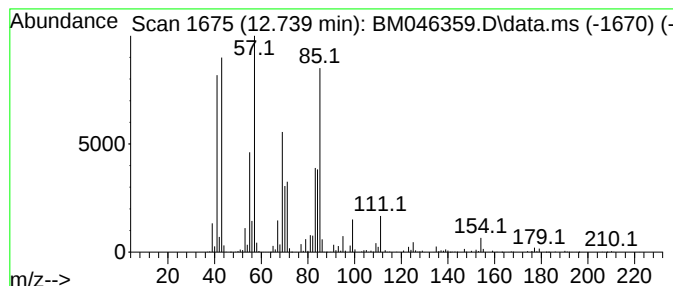
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, 6-ethyloct-3-y... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	25.54 ng	2683710	Acenaphthene-d10	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, 6-ethyloct-3-yl iso...	314	C18H34O4	1000309-34-3	58
2			Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	50
3			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	47
4			tert-Butyldimethylsilyl nitrile	141	C7H15NSi	056522-24-8	47
5			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
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ALS Vial : 16 Sample Multiplier: 1

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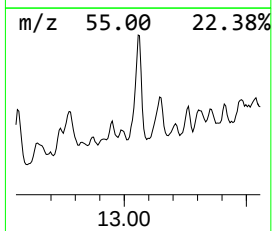
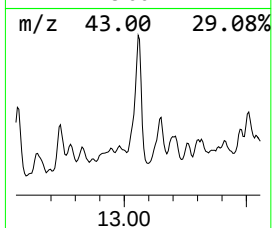
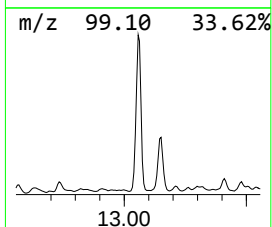
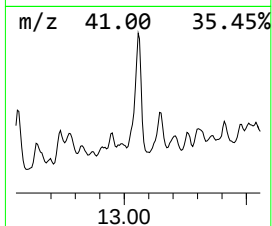
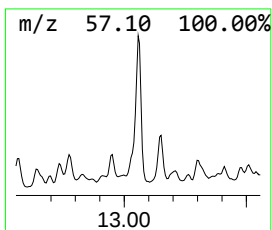
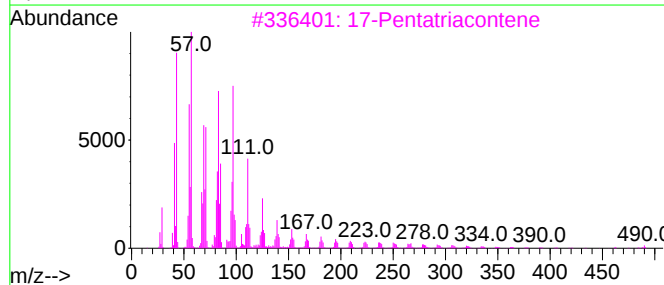
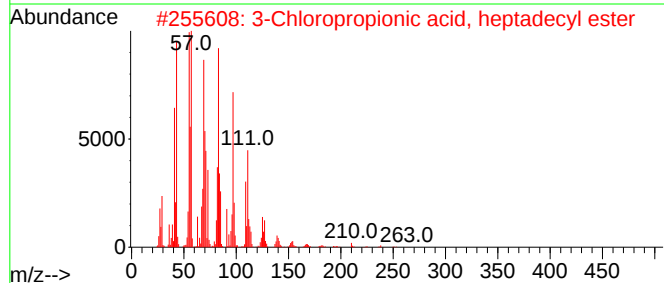
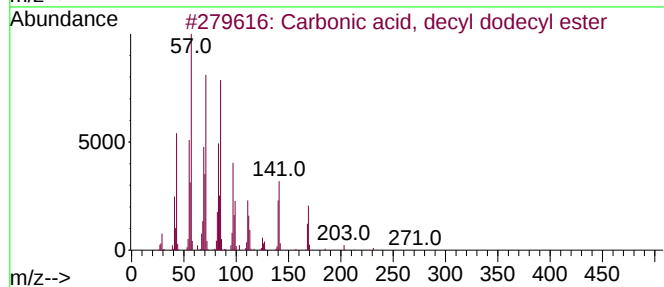
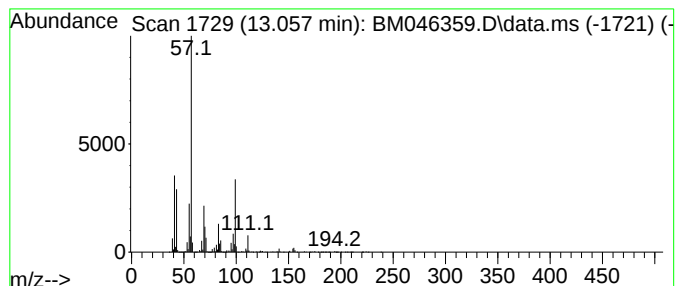
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown13.057 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.057	117.60 ng	12359700	Acenaphthene-d10	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	47
2			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	47
3			17-Pentatriacontene	491	C35H70	006971-40-0	43
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	43
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

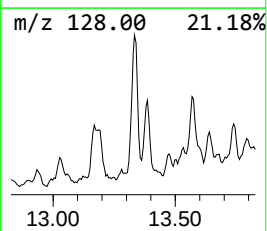
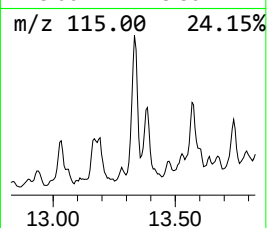
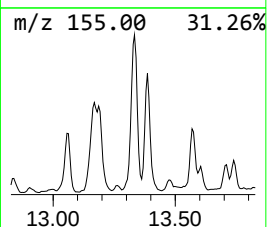
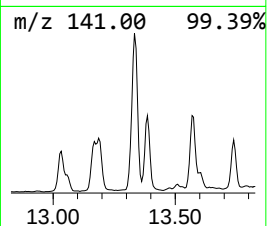
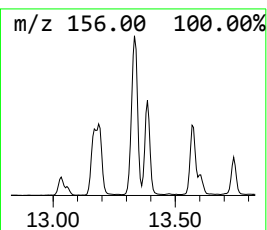
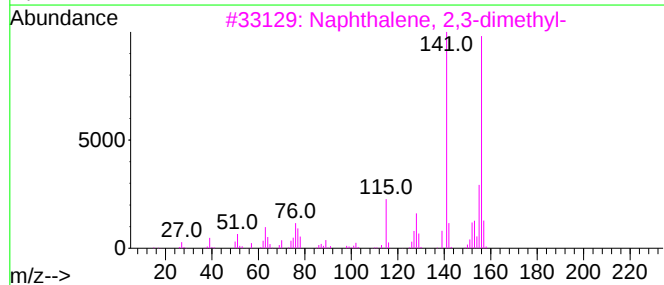
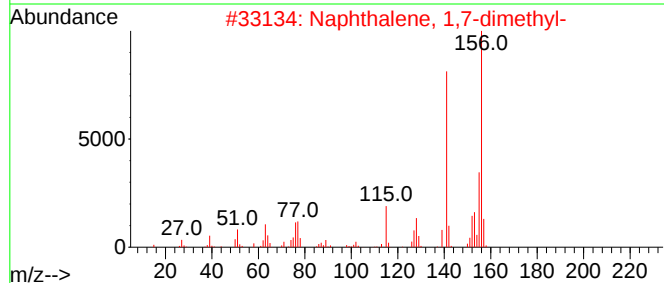
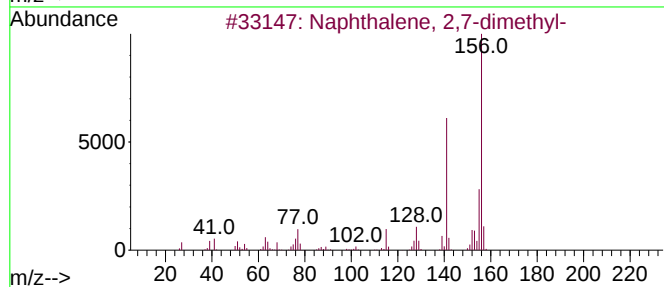
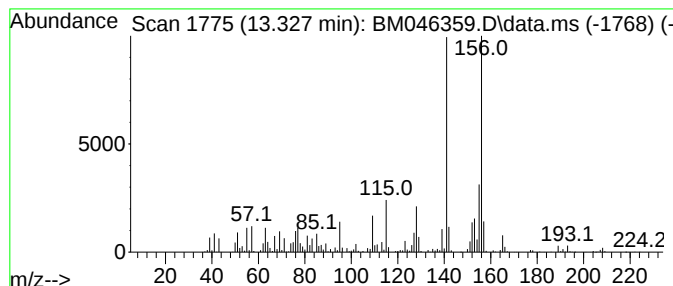
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.327	44.19 ng	4643930	Acenaphthene-d10		14.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-		156	C12H12	000582-16-1	97
2	Naphthalene, 1,7-dimethyl-		156	C12H12	000575-37-1	97
3	Naphthalene, 2,3-dimethyl-		156	C12H12	000581-40-8	97
4	Naphthalene, 2,6-dimethyl-		156	C12H12	000581-42-0	96
5	Naphthalene, 1,8-dimethyl-		156	C12H12	000569-41-5	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
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Sample : P3115-12 2X
Misc :
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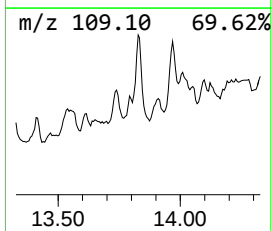
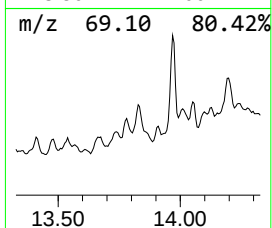
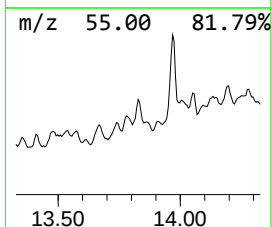
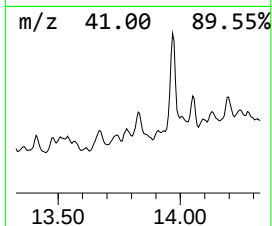
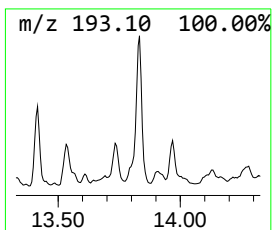
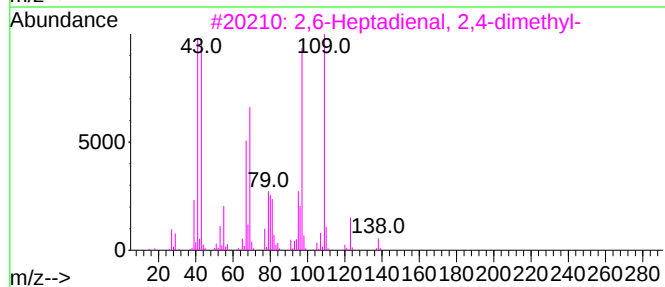
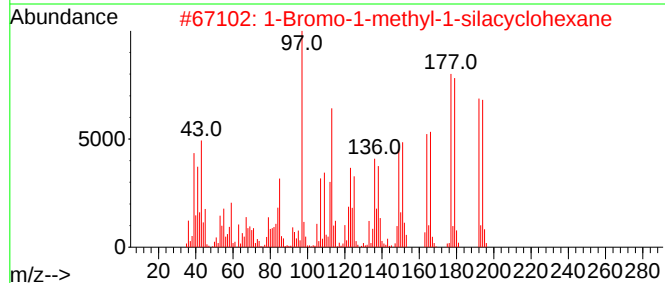
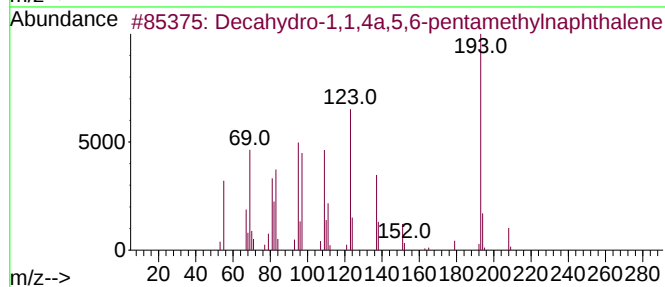
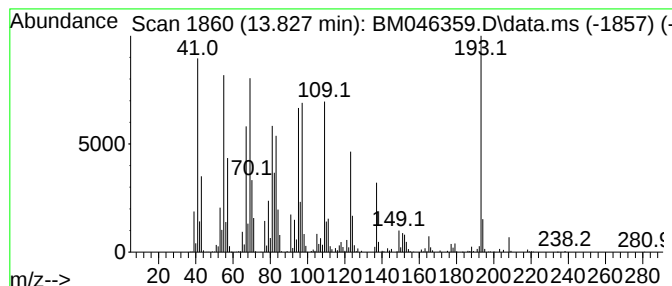
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.827	29.95 ng	3147140	Acenaphthene-d10		14.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	55
2	1-Bromo-1-methyl-1-silacyclohexane		192	C6H13BrSi	085125-32-2	53
3	2,6-Heptadienal, 2,4-dimethyl-		138	C9H14O	085136-08-9	35
4	photocitral B		152	C10H16O	006040-45-5	30
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...		138	C10H18	004863-59-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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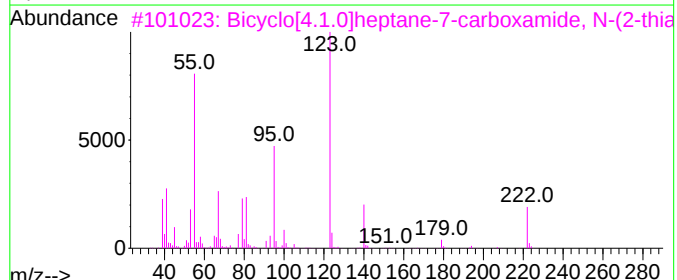
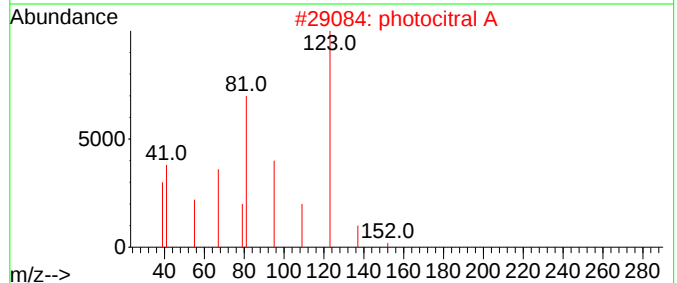
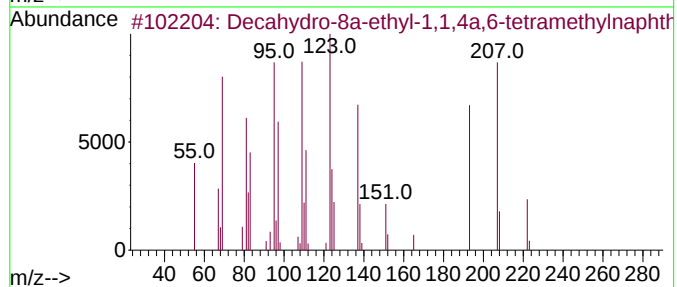
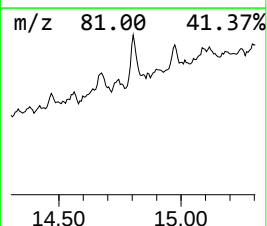
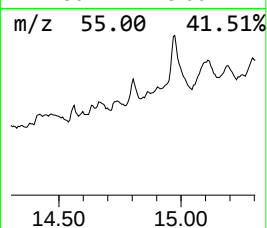
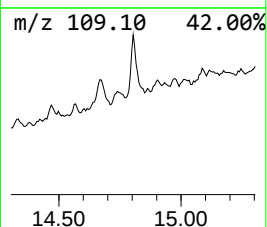
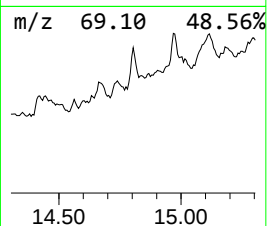
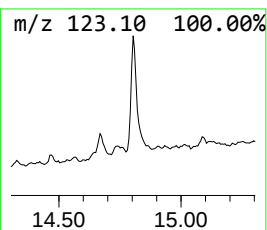
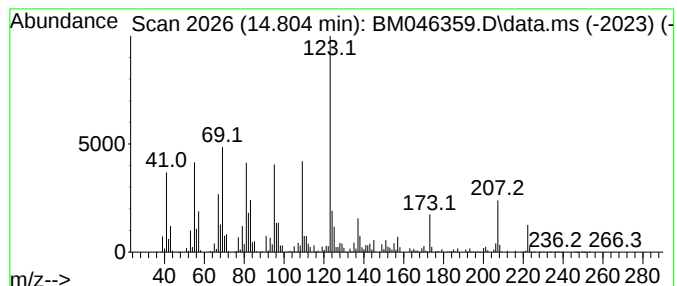
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.804 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	41.75 ng	4387820	Acenaphthene-d10	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	47
2			photocitral A	152	C10H16O	055253-28-6	43
3			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	43
4			2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	43
5			Bicyclo[2.2.2]octane, 1-methyl-4...	202	C10H18O2S	069855-48-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

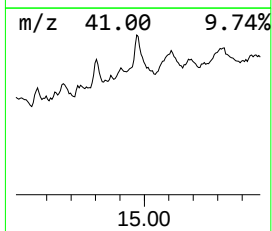
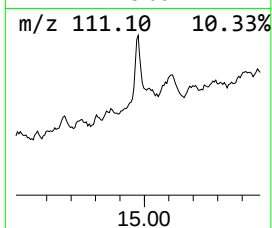
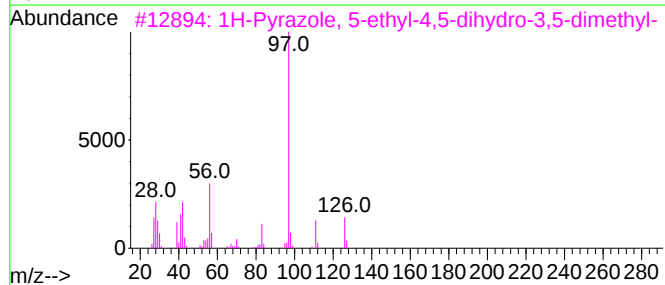
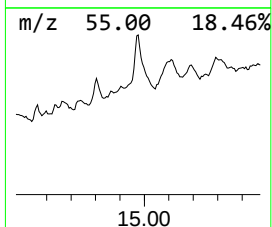
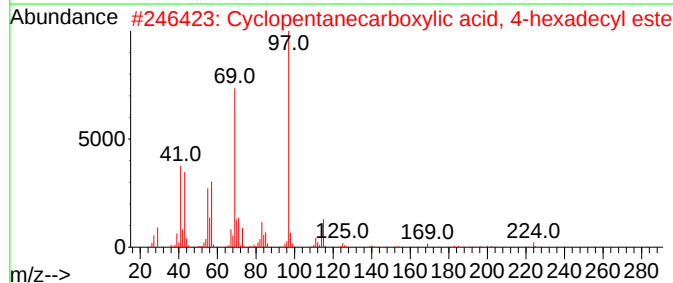
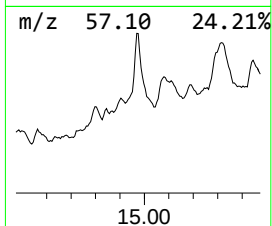
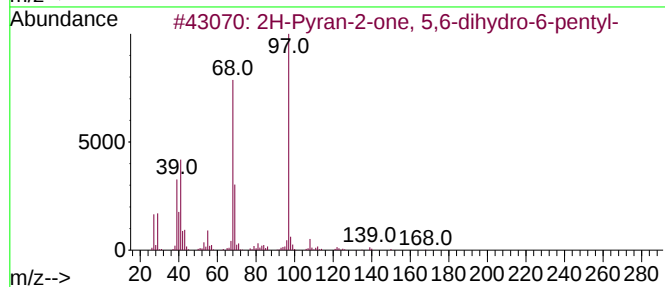
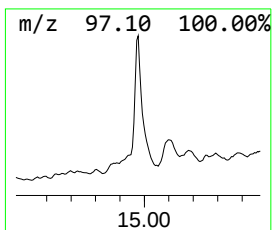
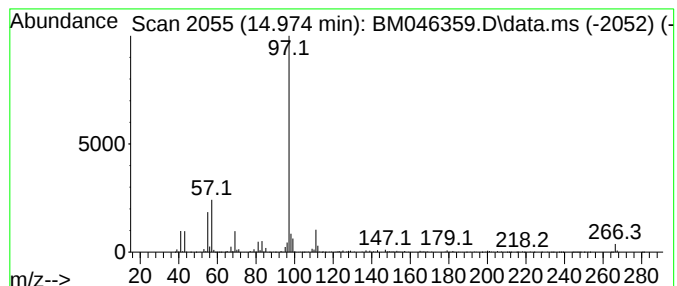
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ClientSampleId :
VNJ-325

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2H-Pyran-2-one, 5,6-dihydro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.974	100.20 ng	10530400	Acenaphthene-d10	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	59
2	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	56
3	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	50
4	2-Thiopheneacetic acid, 1-cyclop...	238	C13H18O2S	1000278-96-0	50
5	5-(2-Thienyl)pentanoic acid	184	C9H12O2S	021010-06-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

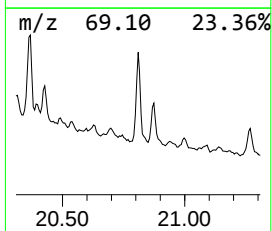
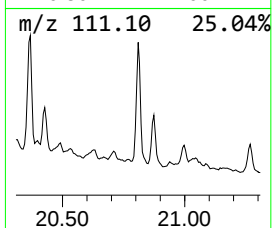
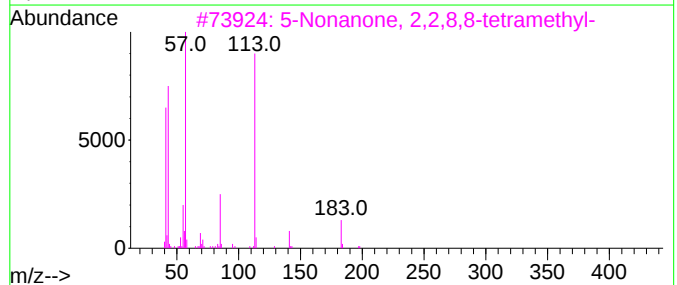
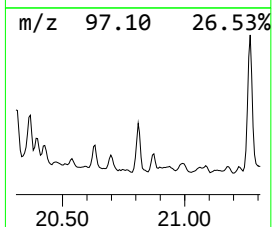
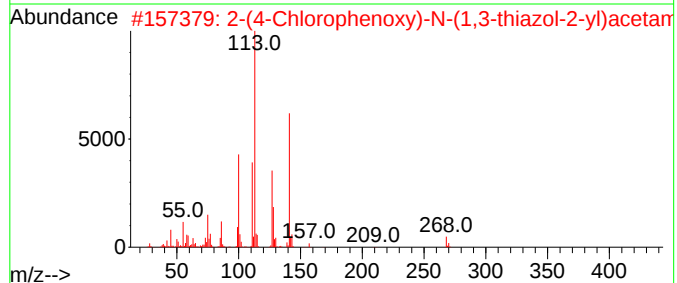
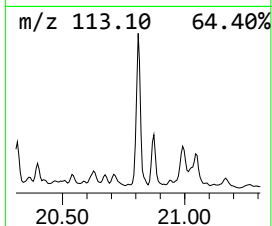
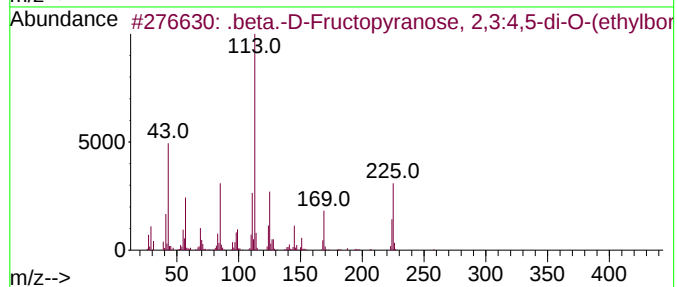
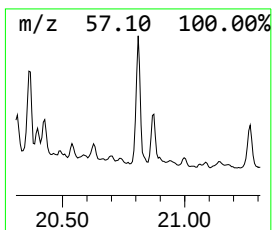
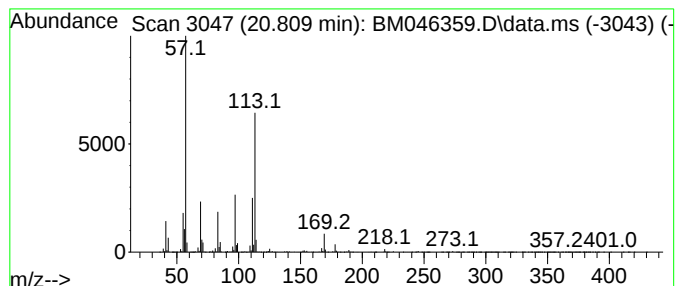
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown20.809 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	19.37 ng	9650650	Chrysene-d12	21.003

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B207	1000156-76-8	38	
2	2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	37		
3	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32		
4	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	27		
5	4-Methylamino-2(5H)-furanone	113	C5H7NO2	1000427-45-5	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-325

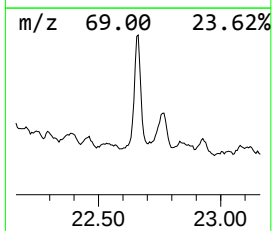
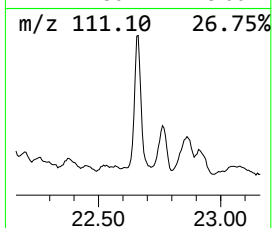
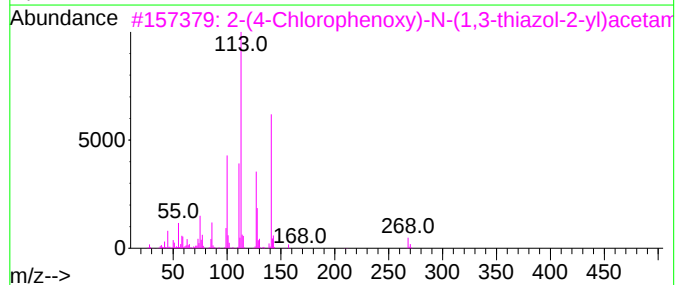
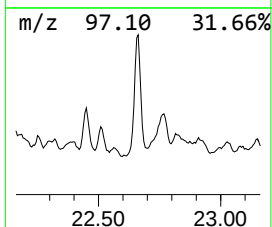
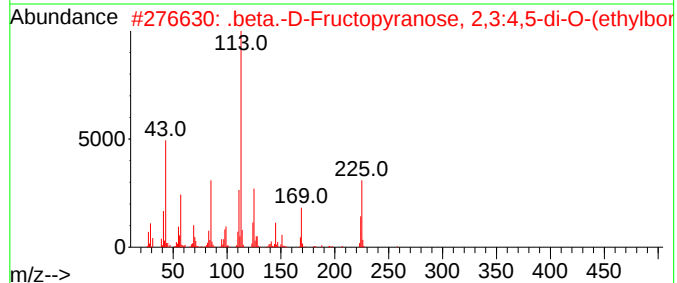
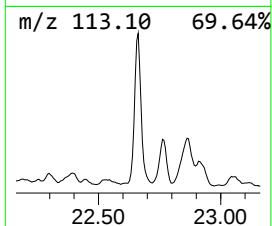
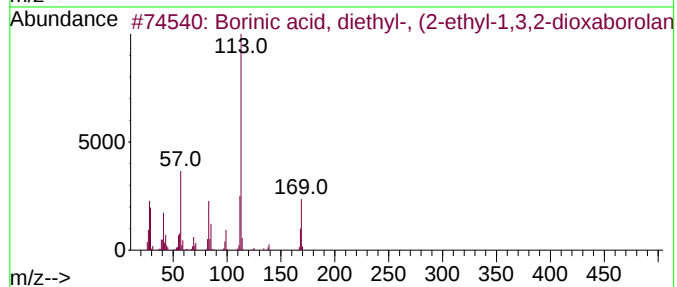
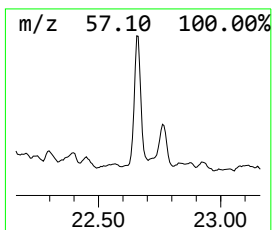
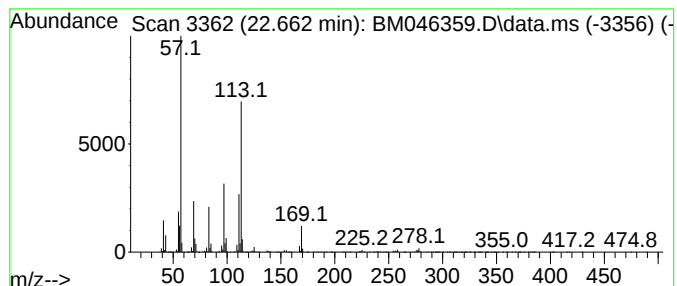
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown22.662 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.662	43.76 ng	6537560	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	37
2			.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	35
3			2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	35
4			Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	35
5			Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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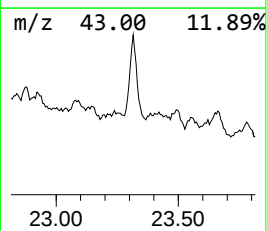
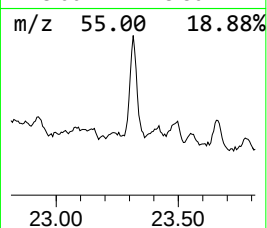
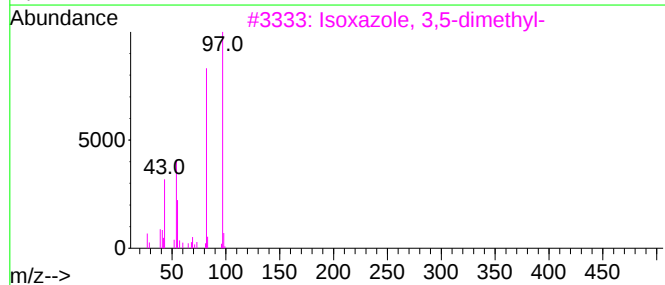
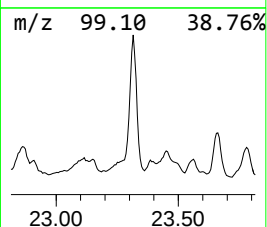
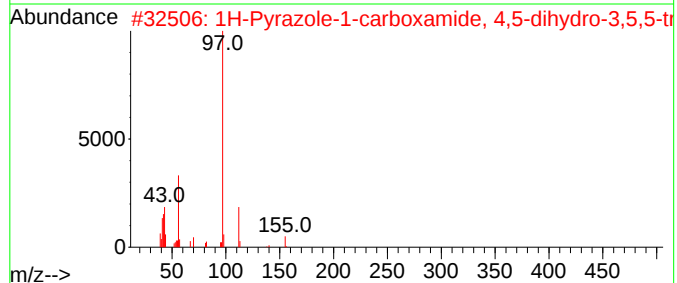
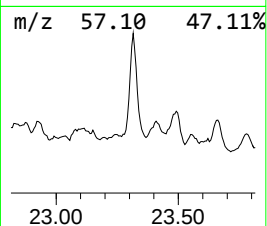
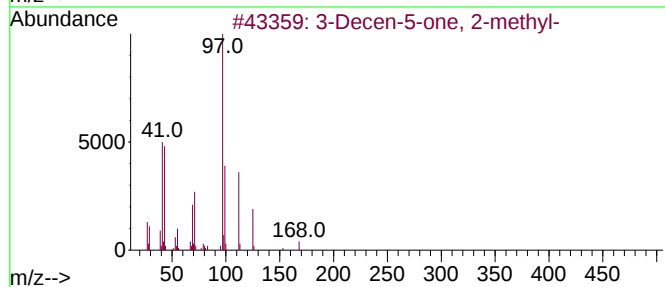
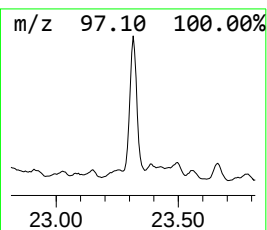
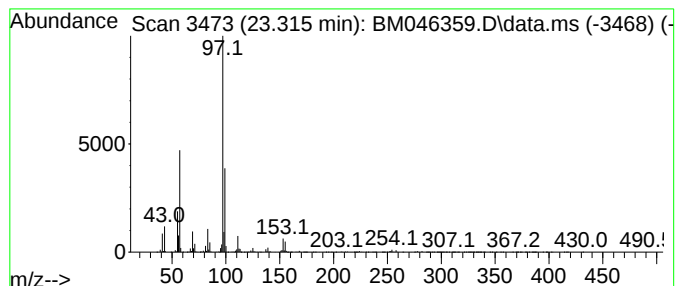
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 3-Decen-5-one, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.315	30.50 ng	4556820	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Decen-5-one, 2-methyl-	168	C11H20O	032064-75-8	59
2			1H-Pyrazole-1-carboxamide, 4,5-d...	155	C7H13N3O	003786-02-5	47
3			Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	47
4			Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	47
5			Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

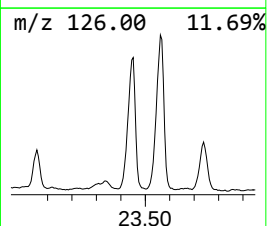
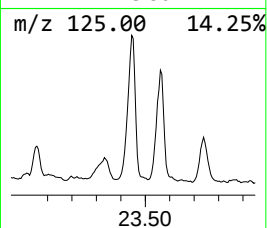
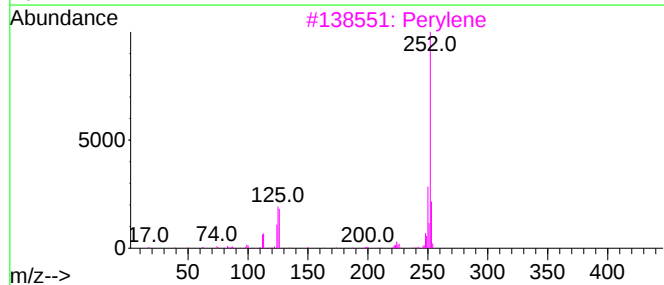
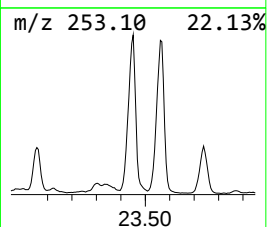
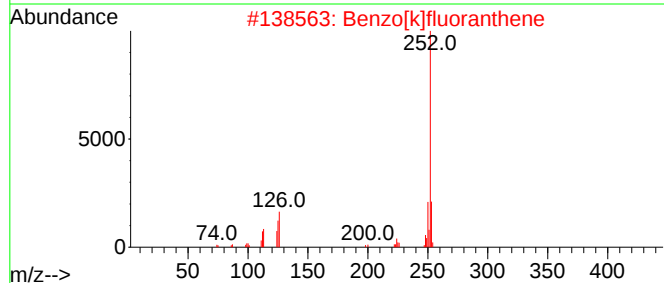
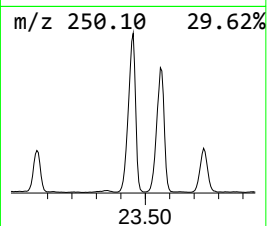
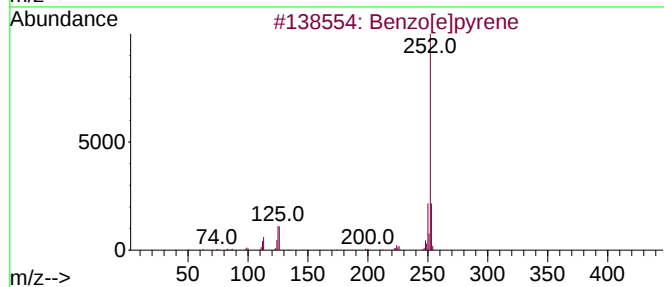
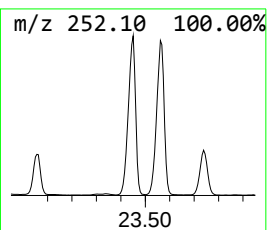
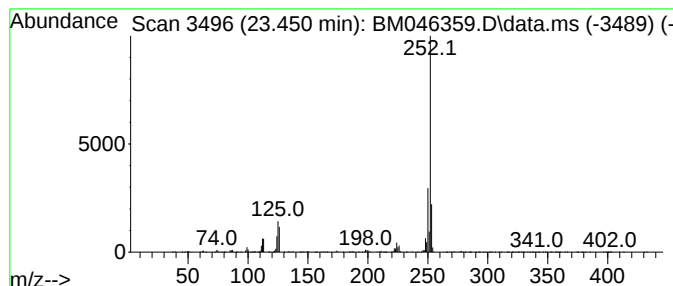
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.450	54.78 ng	8183080	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3			Perylene	252	C20H12	000198-55-0	97
4			Benzo[a]pyrene	252	C20H12	000050-32-8	96
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-325

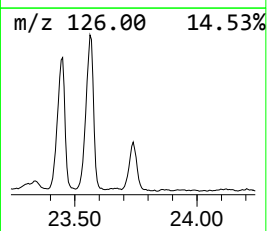
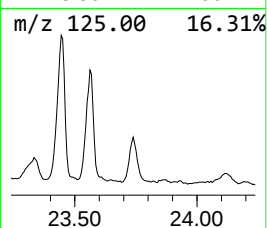
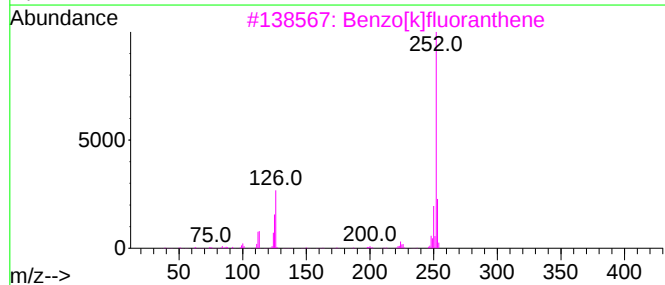
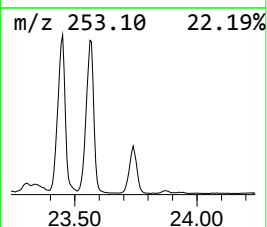
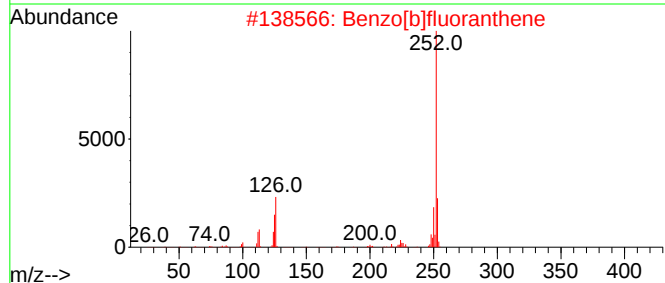
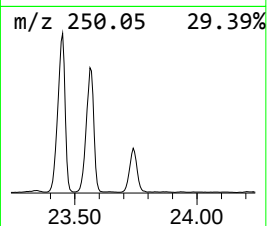
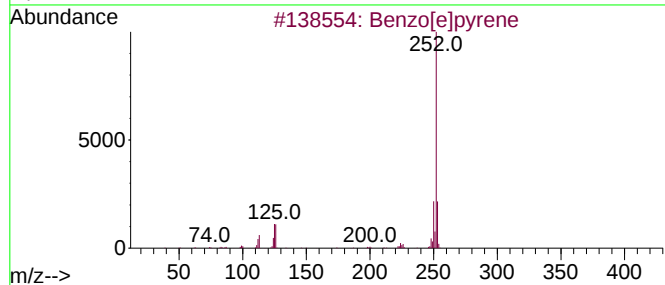
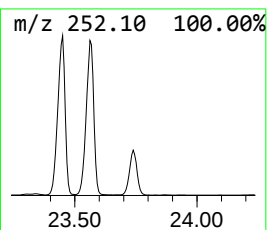
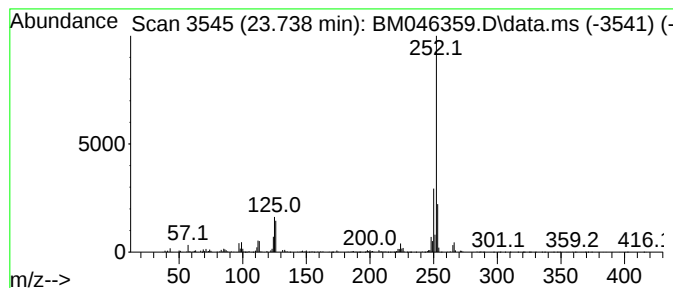
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Perylene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.738	20.00 ng	2987850	Perylene-d12	23.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	97
2		Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4		Perylene	252	C20H12	000198-55-0	96
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
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Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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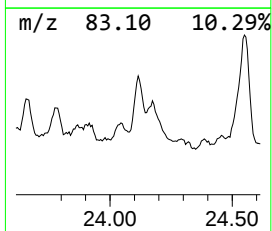
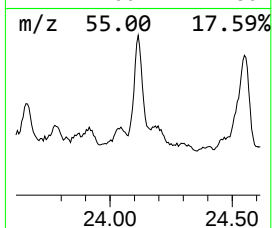
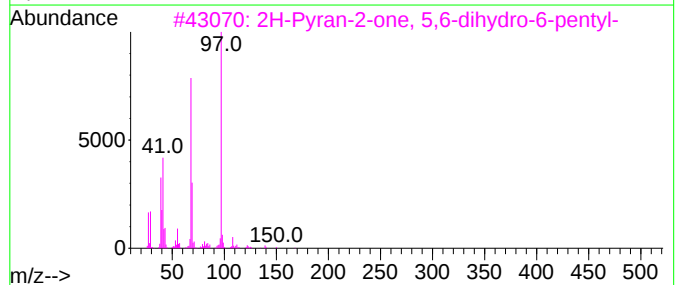
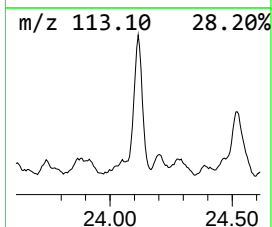
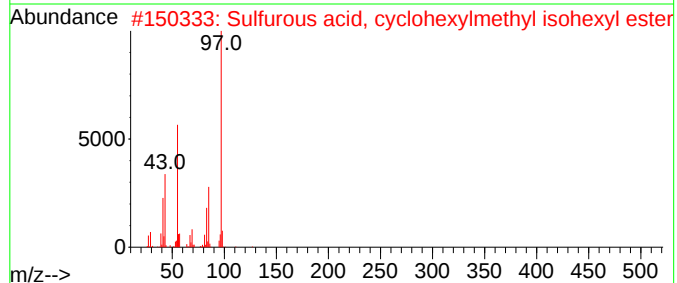
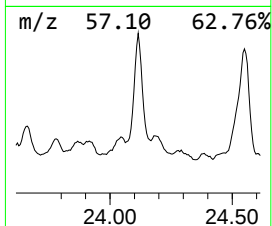
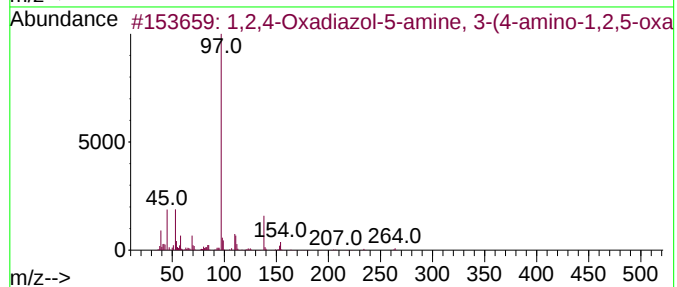
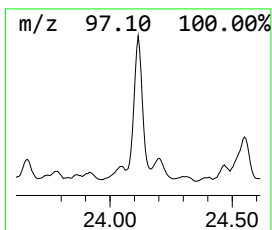
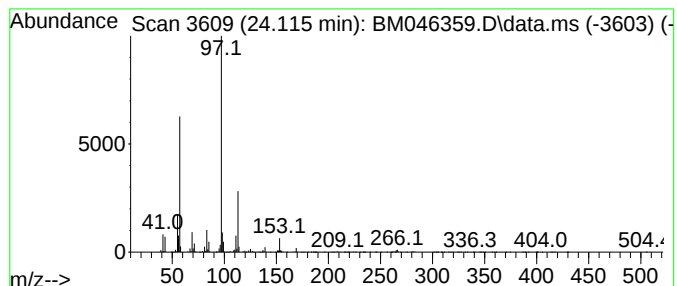
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 1,2,4-Oxadiazol-5-amine, 3-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.115	27.33 ng	4083580	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	53		
2	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	50		
3	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	50		
4	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	50		
5	4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

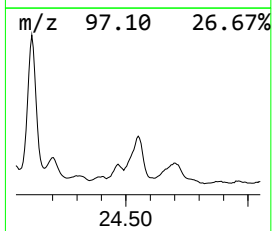
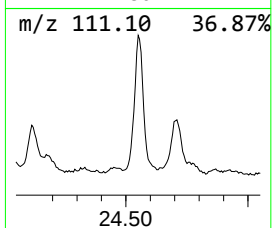
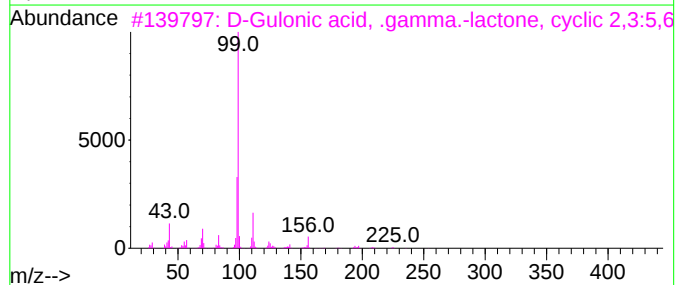
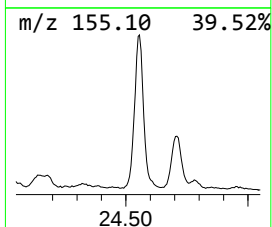
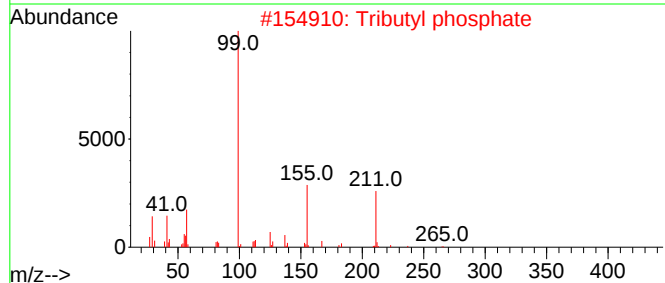
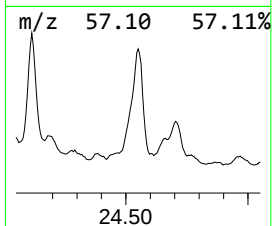
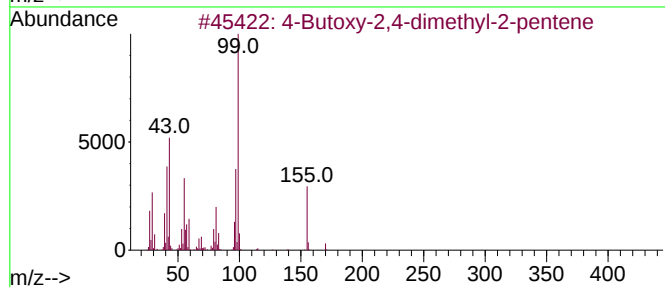
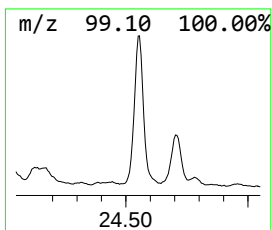
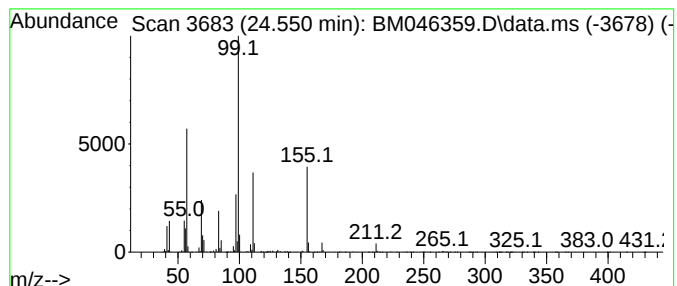
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.550	33.95 ng	5071540	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2			Tributyl phosphate	266	C12H27O4P	000126-73-8	40
3			D-Gulonic acid, .gamma.-lactone,...	254	C10H16B2O6	074128-60-2	37
4			Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	35
5			2,4,4-Trimethyl-1-pentyl methylp...	210	C9H20F02P	333416-06-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

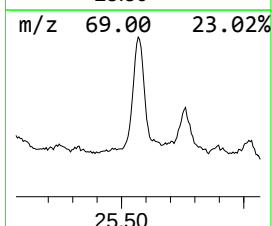
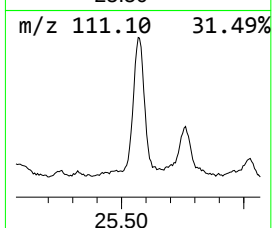
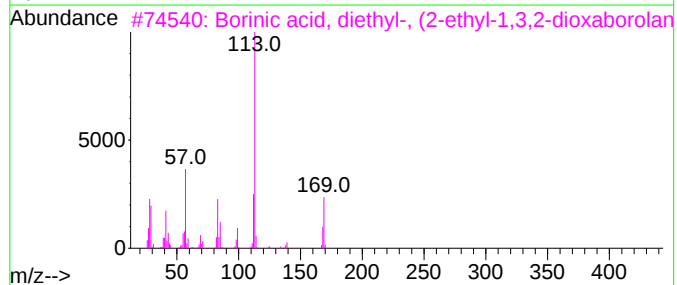
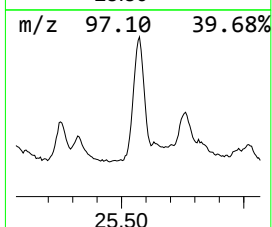
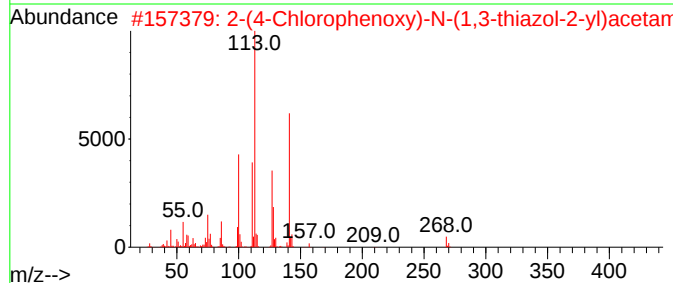
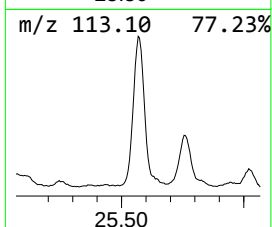
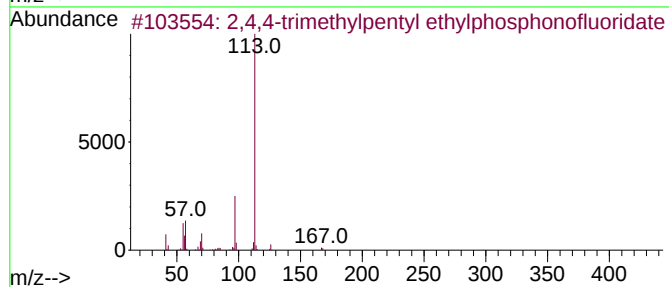
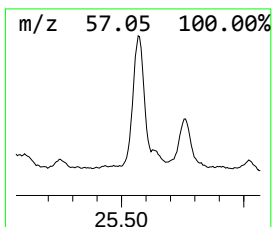
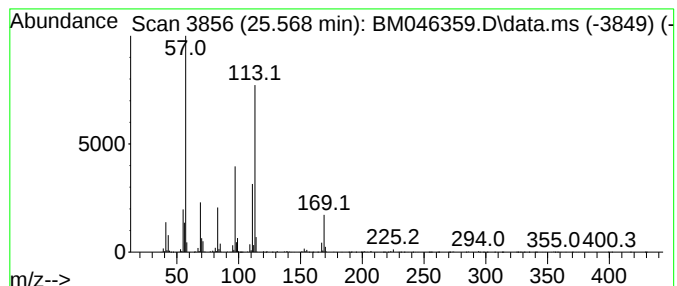
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown25.568 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.568	26.59 ng	3971600	Perylene-d12	23.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-trimethylpentyl ethylphosp...	224	C10H22F02P	333416-13-0	43		
2	2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	38		
3	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	37		
4	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	35		
5	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

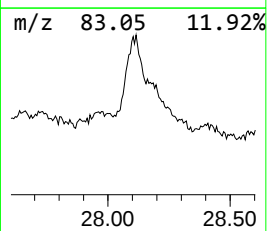
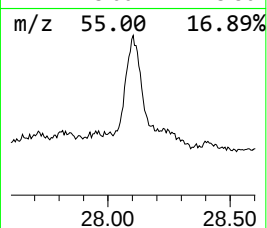
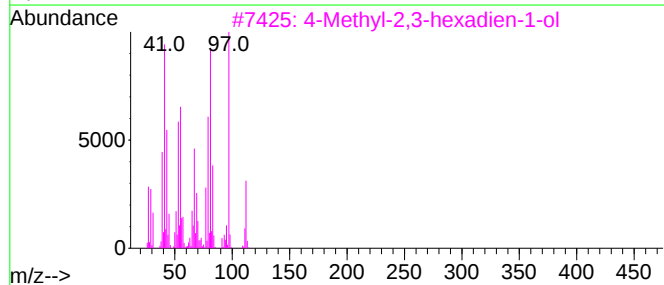
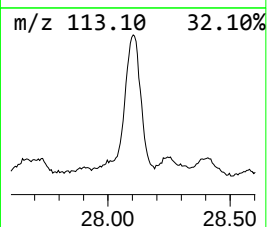
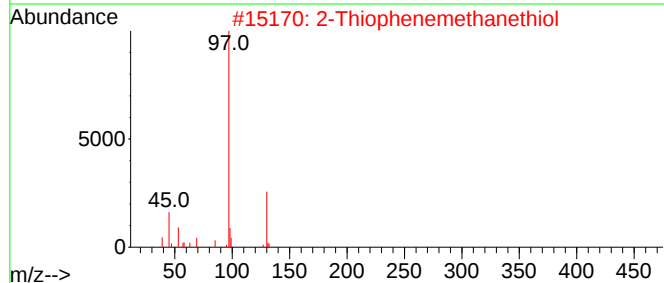
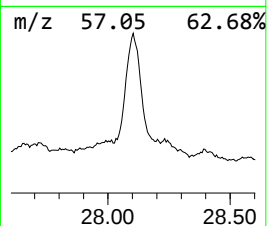
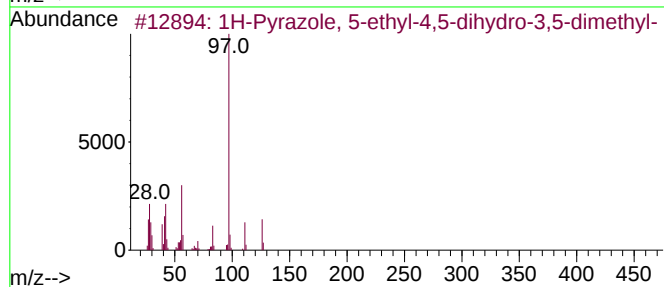
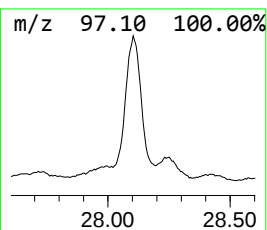
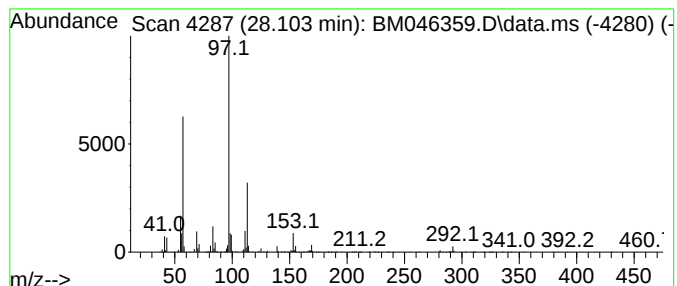
Instrument :
BNA_M
ClientSampleId :
VNJ-325

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 1H-Pyrazole, 5-ethyl-4,5-di... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.103	23.46 ng	3505320	Perylene-d12	23.674	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	53
2	2-Thiophenemethanethiol	130	C5H6S2	006258-63-5	52
3	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	50
4	2-Thiopheneacetic acid, allyl ester	182	C9H10O2S	1000278-98-5	47
5	3-Cyclopent-1-enyl-3-hydroxy-2-m...	170	C9H14O3	1000191-19-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046359.D
Acq On : 28 Jun 2024 19:23
Operator : MA/JU
Sample : P3115-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-325

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentene, 3,4,...	11.357	26.3	ng	1956280	2	10.128	1489450	20.0
3-Heptene, 2,2,...	12.310	19.1	ng	2010850	3	14.015	2101910	20.0
2,4,4,6,6,8,8-H...	12.404	54.0	ng	5677060	3	14.015	2101910	20.0
Hexane, 1-(hexy...	12.510	38.3	ng	4023070	3	14.015	2101910	20.0
Sulfurous acid,...	12.569	43.0	ng	4517190	3	14.015	2101910	20.0
Oxalic acid, 6-...	12.739	25.5	ng	2683710	3	14.015	2101910	20.0
unknown13.057	13.057	117.6	ng	12359700	3	14.015	2101910	20.0
Naphthalene, 2,...	13.327	44.2	ng	4643930	3	14.015	2101910	20.0
Decahydro-1,1,4...	13.827	29.9	ng	3147140	3	14.015	2101910	20.0
unknown14.804	14.804	41.8	ng	4387820	3	14.015	2101910	20.0
2H-Pyran-2-one,...	14.974	100.2	ng	10530400	3	14.015	2101910	20.0
unknown20.809	20.809	19.4	ng	9650650	5	21.003	9964620	20.0
unknown22.662	22.662	43.8	ng	6537560	6	23.674	2987850	20.0
3-Decen-5-one, ...	23.315	30.5	ng	4556820	6	23.674	2987850	20.0
Benzo[e]pyrene	23.450	54.8	ng	8183080	6	23.674	2987850	20.0
Perylene	23.738	20.0	ng	2987850	6	23.674	2987850	20.0
1,2,4-Oxadiazol...	24.115	27.3	ng	4083580	6	23.674	2987850	20.0
4-Butoxy-2,4-di...	24.550	34.0	ng	5071540	6	23.674	2987850	20.0
unknown25.568	25.568	26.6	ng	3971600	6	23.674	2987850	20.0
1H-Pyrazole, 5-...	28.103	23.5	ng	3505320	6	23.674	2987850	20.0