

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
 Data File : BF137030.D
 Acq On : 10 Jan 2024 20:33
 Operator : CG\JU
 Sample : P1068-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-01-010824

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_F\Methods\8270-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	5	8	13	rVB2	12673	17281	2.10%	0.203%
2	4.440	395	400	406	rVB5	7369	12492	1.52%	0.147%
3	5.016	490	498	505	rBV2	39423	57626	7.02%	0.676%
4	5.204	526	530	532	rBV	12420	12718	1.55%	0.149%
5	5.381	558	560	565	rVB2	11091	11373	1.38%	0.133%
6	5.428	565	568	583	rBV	799488	810847	98.71%	9.514%
7	5.698	611	614	619	rVB	13727	13231	1.61%	0.155%
8	5.810	627	633	637	rBV	8456	10580	1.29%	0.124%
9	6.034	666	671	677	rBV3	7714	10945	1.33%	0.128%
10	6.310	715	718	723	rBV2	11116	12002	1.46%	0.141%
11	6.434	736	739	751	rBV	820349	778049	94.72%	9.129%
12	6.616	766	770	772	rBV2	25863	25113	3.06%	0.295%
13	6.787	795	799	803	rVB	302384	258353	31.45%	3.031%
14	7.045	838	843	847	rBV3	11334	15601	1.90%	0.183%
15	7.163	859	863	867	rBV3	8274	10917	1.33%	0.128%
16	7.345	891	894	897	rBV	610638	479884	58.42%	5.631%
17	7.369	897	898	902	rVV	33185	28585	3.48%	0.335%
18	7.422	902	907	910	rVB6	11434	16487	2.01%	0.193%
19	7.481	910	917	920	rBV6	5657	13170	1.60%	0.155%
20	7.810	969	973	977	rBV6	10796	18365	2.24%	0.215%
21	8.039	1009	1012	1013	rBV	36268	27988	3.41%	0.328%
22	8.063	1013	1016	1018	rVV	359359	300028	36.53%	3.520%
23	8.081	1018	1019	1023	rVV	44035	37652	4.58%	0.442%
24	8.116	1023	1025	1028	rVB	23964	18409	2.24%	0.216%
25	8.257	1046	1049	1052	rVB3	13054	11999	1.46%	0.141%
26	8.351	1060	1065	1071	rBV7	13447	19249	2.34%	0.226%
27	8.434	1077	1079	1083	rVB5	10047	11027	1.34%	0.129%
28	8.481	1083	1087	1088	rBV	29154	24024	2.92%	0.282%
29	8.598	1103	1107	1109	rBV3	9122	10891	1.33%	0.128%
30	8.651	1112	1116	1119	rBV	28635	26553	3.23%	0.312%
31	8.745	1128	1132	1135	rVB6	12646	16339	1.99%	0.192%
32	8.775	1135	1137	1140	rBV	29242	25692	3.13%	0.301%
33	8.875	1151	1154	1157	rVB	25999	22361	2.72%	0.262%
34	8.934	1161	1164	1167	rBV4	9272	12429	1.51%	0.146%
35	9.010	1174	1177	1181	rBV2	7922	11027	1.34%	0.129%
36	9.081	1186	1189	1193	rVB	33584	29150	3.55%	0.342%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.139	1195	1199	1202	rBV	938023	816252	99.37%	9.577%
38	9.216	1208	1212	1215	rBV	38276	34627	4.22%	0.406%
39	9.404	1241	1244	1247	rVB3	19810	23619	2.88%	0.277%
40	9.475	1253	1256	1259	rBV	29284	32220	3.92%	0.378%
41	9.522	1262	1264	1265	rVV2	19959	19056	2.32%	0.224%
42	9.539	1265	1267	1269	rVB2	28123	21703	2.64%	0.255%
43	9.592	1274	1276	1280	rVB3	15741	13657	1.66%	0.160%
44	9.681	1287	1291	1295	rBV2	34607	33310	4.06%	0.391%
45	9.722	1295	1298	1300	rVV2	16727	14341	1.75%	0.168%
46	9.745	1300	1302	1306	rVB	28799	23350	2.84%	0.274%
47	9.816	1311	1314	1318	rVV	345339	304248	37.04%	3.570%
48	9.851	1318	1320	1325	rVV	24095	23753	2.89%	0.279%
49	9.928	1329	1333	1337	rVB5	12191	19202	2.34%	0.225%
50	9.975	1337	1341	1345	rBV7	10325	22159	2.70%	0.260%
51	10.022	1347	1349	1353	rVV3	17009	19836	2.41%	0.233%
52	10.063	1353	1356	1361	rVB3	16819	17270	2.10%	0.203%
53	10.133	1365	1368	1372	rBV3	13487	17896	2.18%	0.210%
54	10.222	1379	1383	1385	rBV4	13606	15958	1.94%	0.187%
55	10.245	1385	1387	1390	rVB	24962	21010	2.56%	0.247%
56	10.369	1404	1408	1414	rVB2	27694	34251	4.17%	0.402%
57	10.469	1421	1425	1432	rVB2	18998	29549	3.60%	0.347%
58	10.528	1432	1435	1438	rVB4	8475	11680	1.42%	0.137%
59	10.616	1446	1450	1460	rVB	560189	506990	61.72%	5.949%
60	10.733	1465	1470	1474	rBV4	40875	58093	7.07%	0.682%
61	10.916	1498	1501	1504	rBV3	13980	17233	2.10%	0.202%
62	10.951	1504	1507	1509	rVB	13192	11106	1.35%	0.130%
63	11.175	1542	1545	1547	rBV	20707	18055	2.20%	0.212%
64	11.204	1547	1550	1555	rVB2	34611	37808	4.60%	0.444%
65	11.316	1565	1569	1571	rBV	339994	332124	40.43%	3.897%
66	11.339	1571	1573	1576	rVV	134725	110246	13.42%	1.294%
67	11.386	1578	1581	1584	rVV	35787	34550	4.21%	0.405%
68	11.427	1585	1588	1594	rVV8	11716	17258	2.10%	0.202%
69	11.557	1607	1610	1614	rBV2	12714	13482	1.64%	0.158%
70	11.604	1615	1618	1621	rVV2	24823	20626	2.51%	0.242%
71	11.645	1623	1625	1630	rVB3	13477	15182	1.85%	0.178%
72	11.775	1644	1647	1651	rBV6	10045	15053	1.83%	0.177%
73	11.816	1651	1654	1657	rVV	32910	39805	4.85%	0.467%
74	11.845	1657	1659	1664	rVV	123516	125804	15.32%	1.476%
75	11.892	1665	1667	1670	rVV2	22401	29213	3.56%	0.343%
76	11.927	1670	1673	1676	rVV	51216	66015	8.04%	0.775%

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Integrator: RTE

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77	11.951	1676	1677	1680	rVB	29398	19446	2.37%	0.228%
78	12.010	1685	1687	1692	rVV	21741	21162	2.58%	0.248%
79	12.292	1733	1735	1738	rBV	23005	21425	2.61%	0.251%
80	12.369	1745	1748	1750	rBV2	38547	36768	4.48%	0.431%
81	12.404	1750	1754	1761	rVB4	50974	84971	10.34%	0.997%
82	12.457	1761	1763	1768	rBV6	16946	30537	3.72%	0.358%
83	12.533	1773	1776	1780	rBV	228609	202941	24.71%	2.381%
84	12.763	1810	1815	1822	rBV	219957	259451	31.59%	3.044%
85	12.821	1822	1825	1829	rBV6	28326	36648	4.46%	0.430%
86	12.910	1836	1840	1843	rBV	949279	821423	100.00%	9.638%
87	13.139	1876	1879	1881	rBV3	39345	39475	4.81%	0.463%
88	13.163	1881	1883	1886	rVV	27051	26530	3.23%	0.311%
89	13.480	1935	1937	1940	rBV2	39036	35727	4.35%	0.419%
90	13.974	2017	2021	2024	rBV2	368204	400636	48.77%	4.701%
91	15.468	2272	2275	2281	rVB	183400	229679	27.96%	2.695%

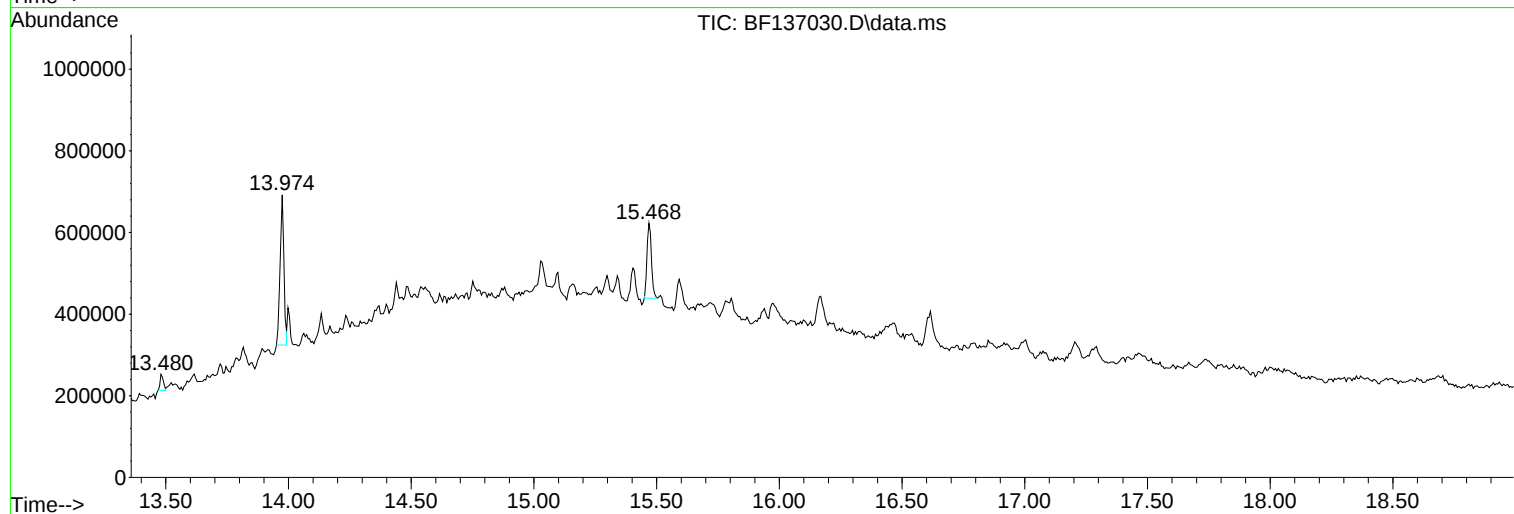
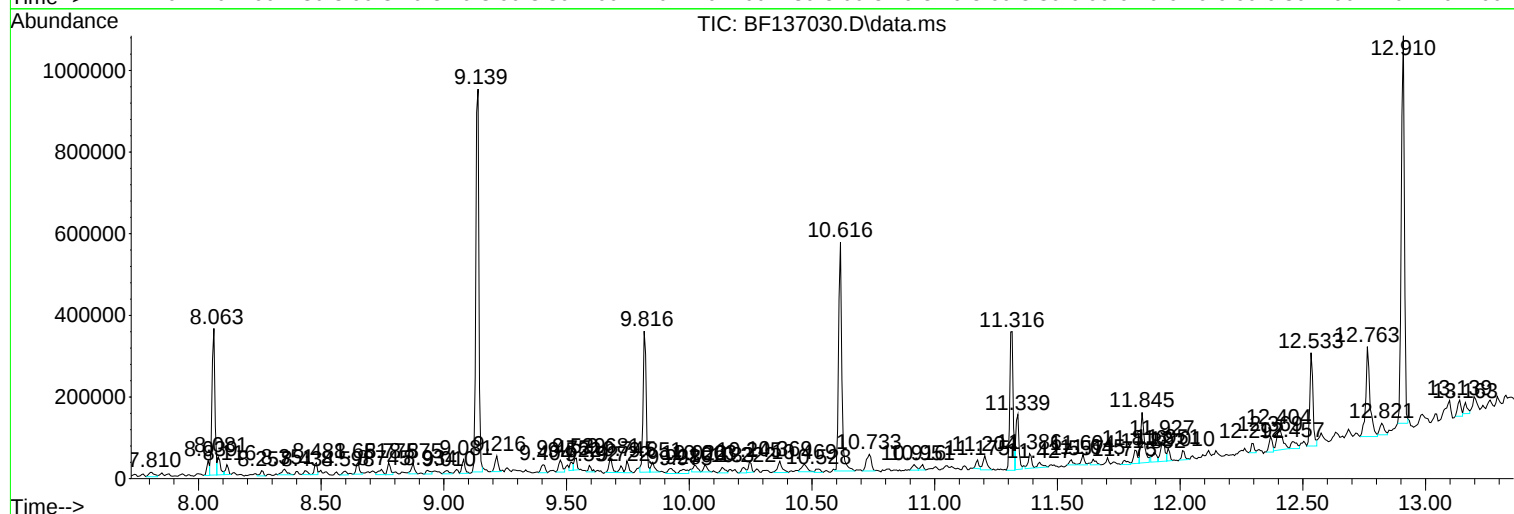
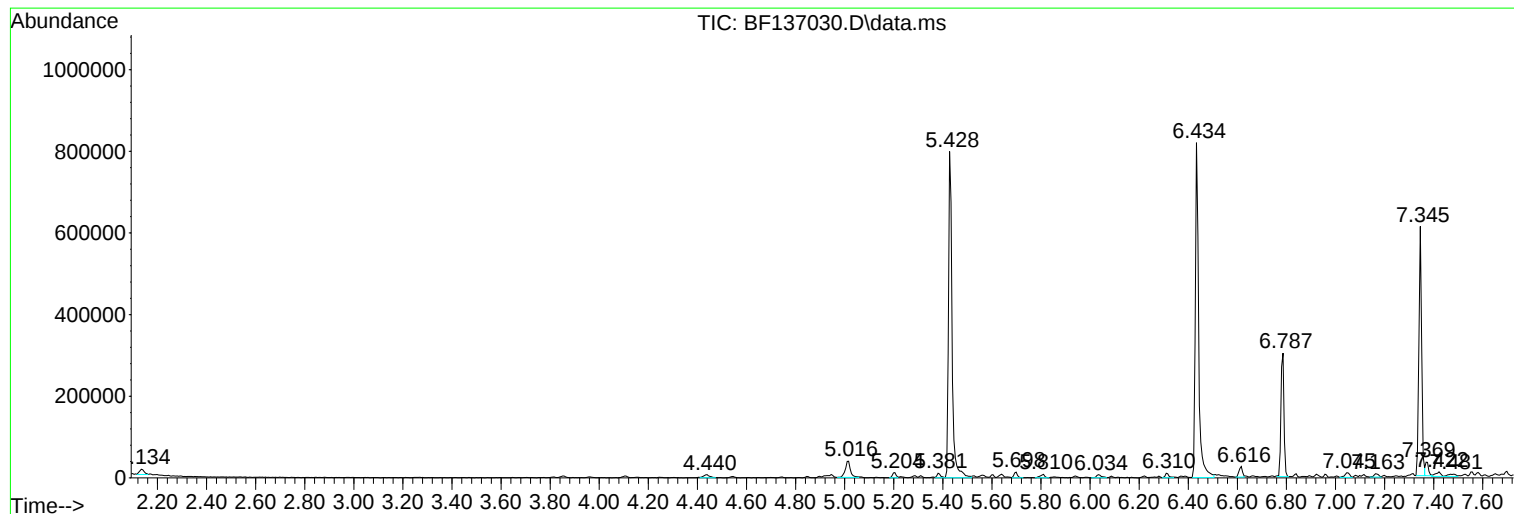
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-010824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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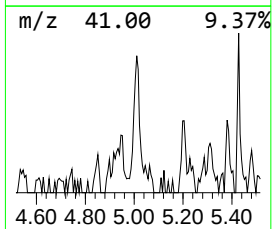
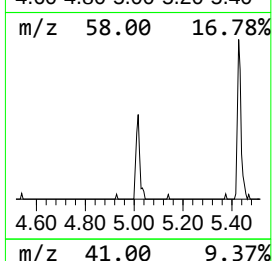
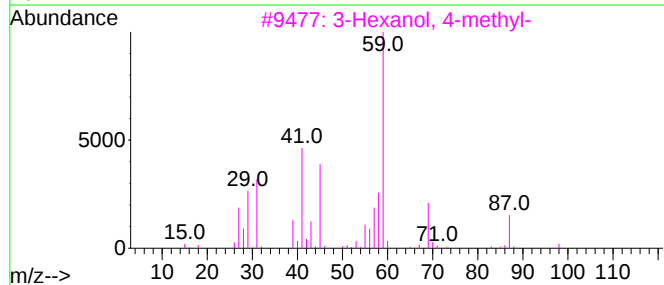
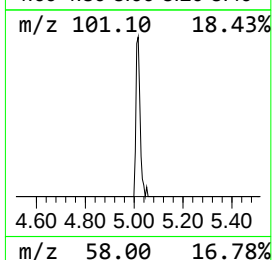
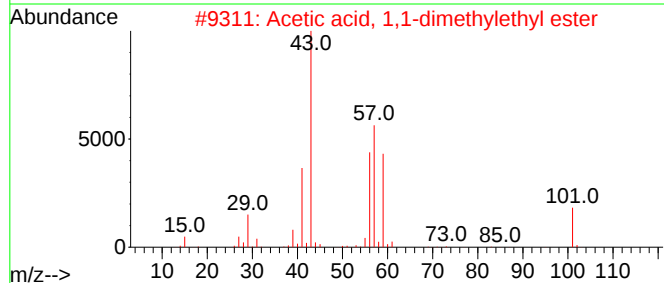
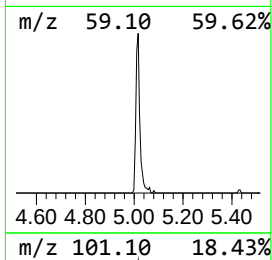
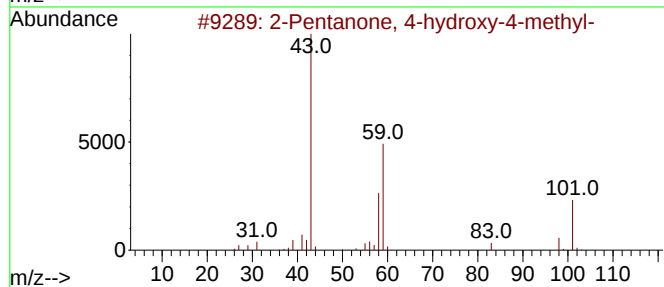
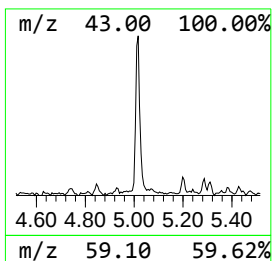
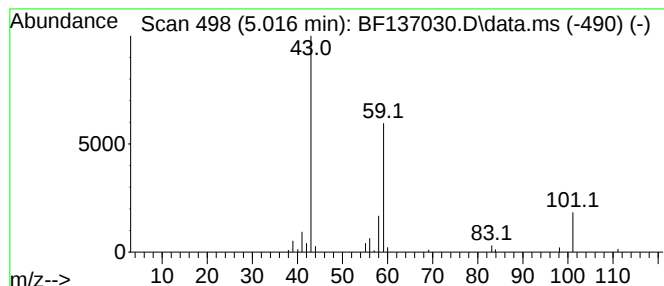
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	4.46 ng	57626	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		



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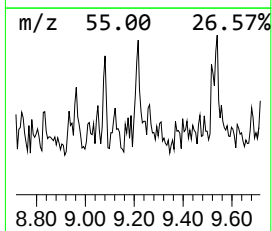
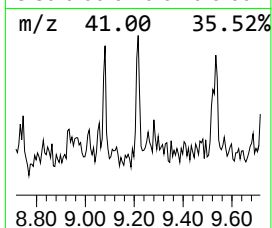
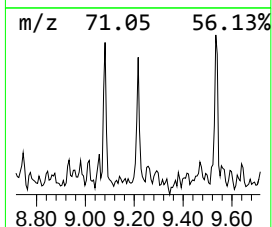
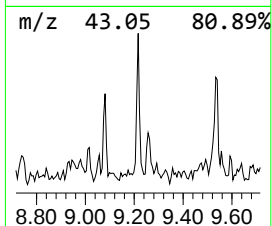
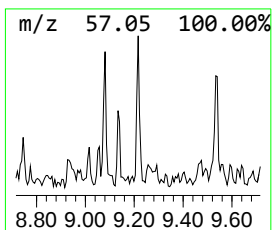
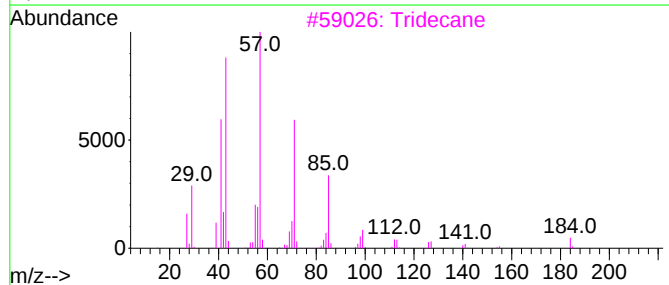
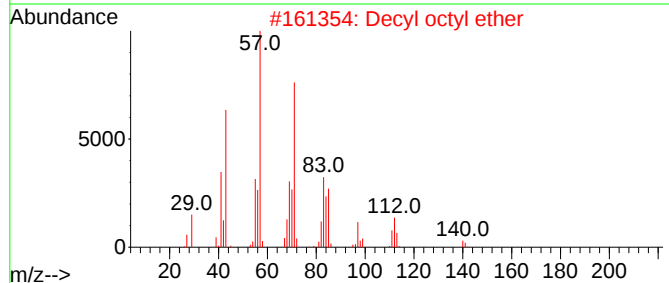
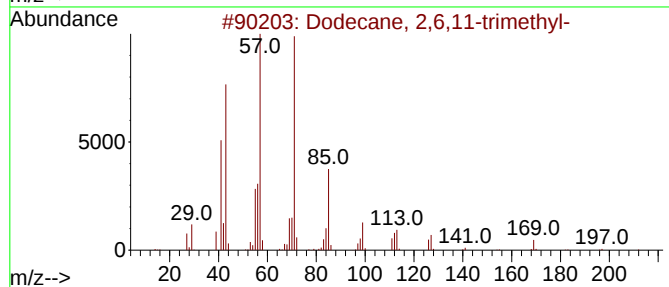
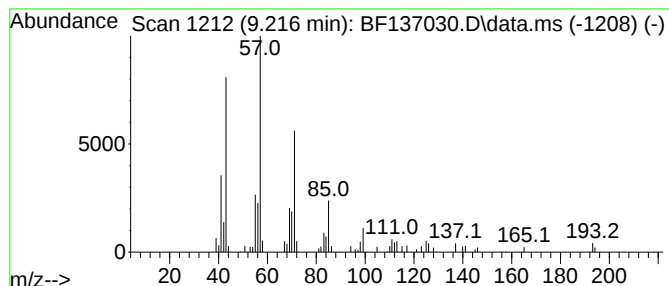
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 2,6,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	2.28 ng	34627	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
2			Decyl octyl ether	270	C18H38O	1000406-38-3	64
3			Tridecane	184	C13H28	000629-50-5	64
4			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	64
5			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	59



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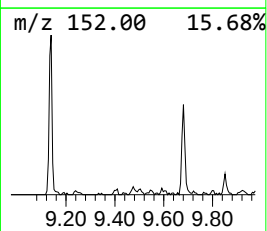
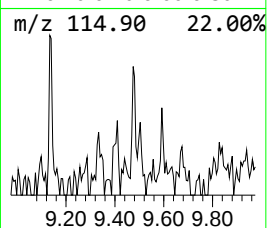
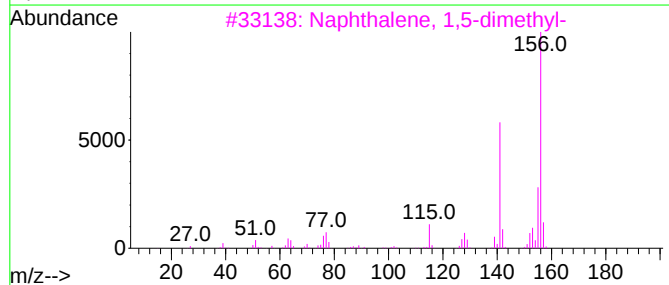
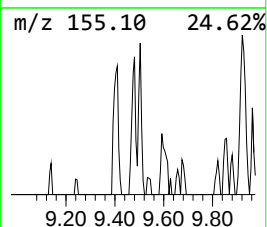
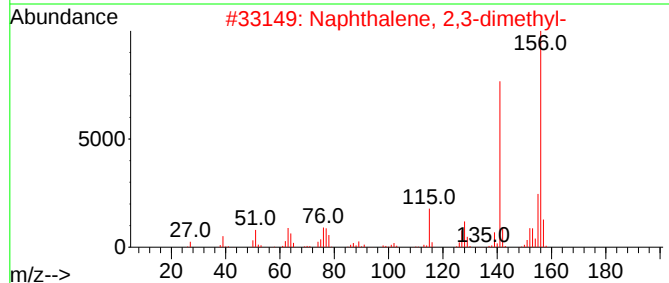
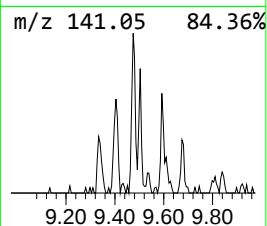
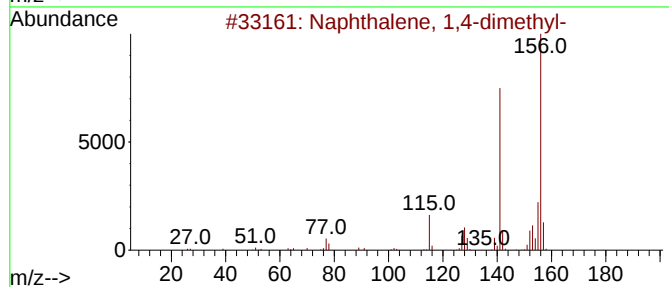
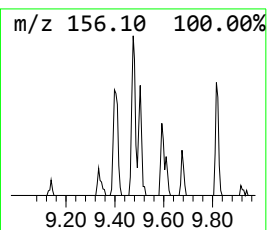
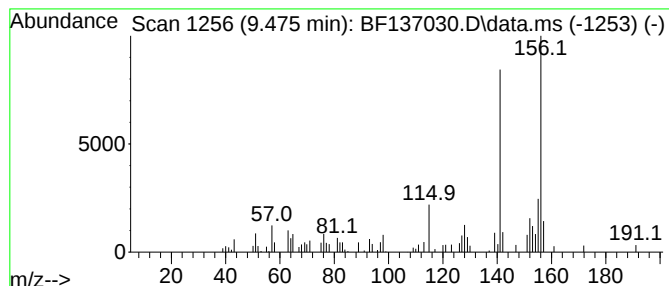
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1,4-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.475	2.12 ng	32220	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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Acq On : 10 Jan 2024 20:33
Operator : CG\JU
Sample : P1068-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CL-01-010824

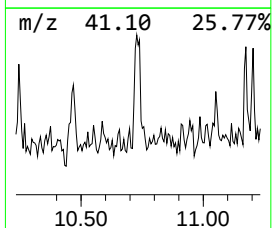
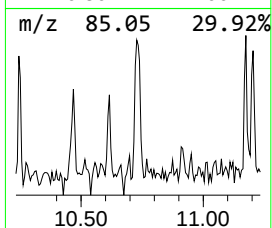
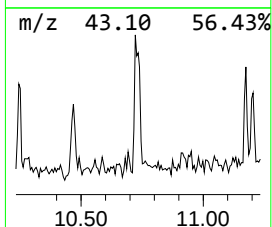
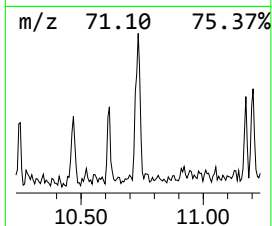
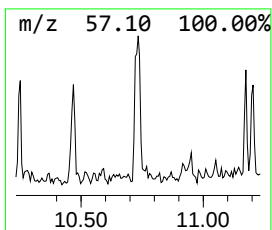
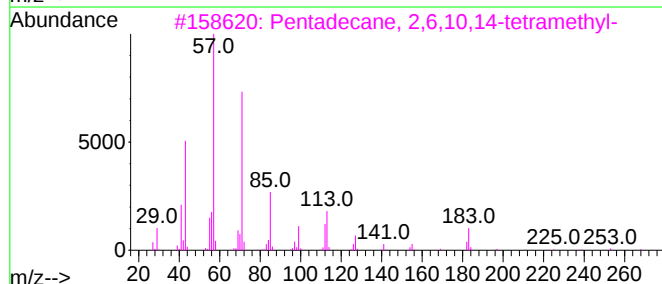
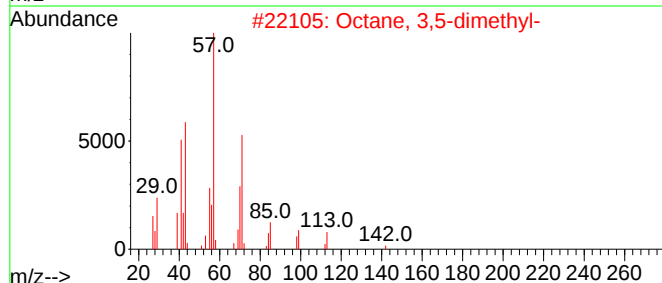
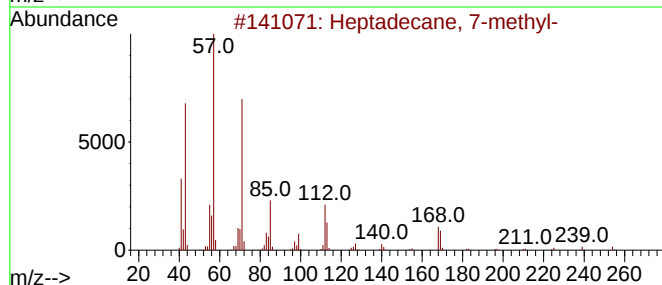
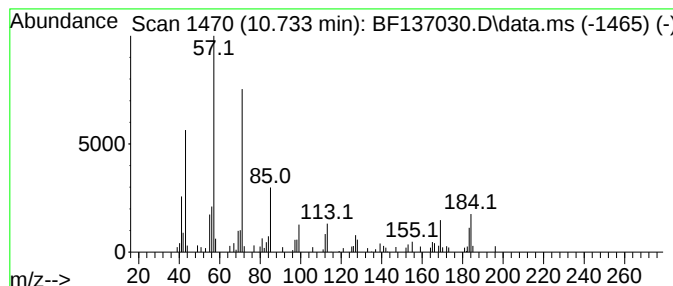
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 7-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	3.50 ng	58093	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	80
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	68
3			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	64
4			Decane, 2-methyl-	156	C11H24	006975-98-0	59
5			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137030.D
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ClientSampleId :
CL-01-010824

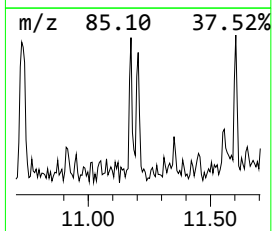
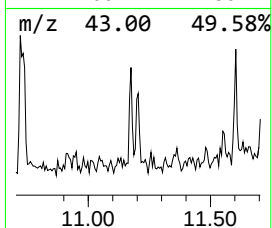
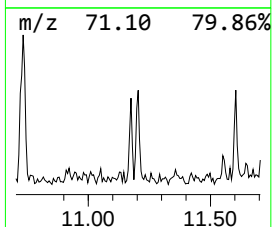
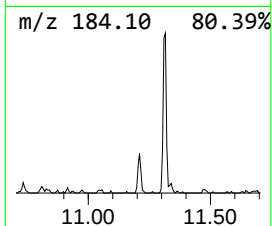
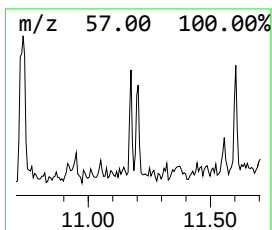
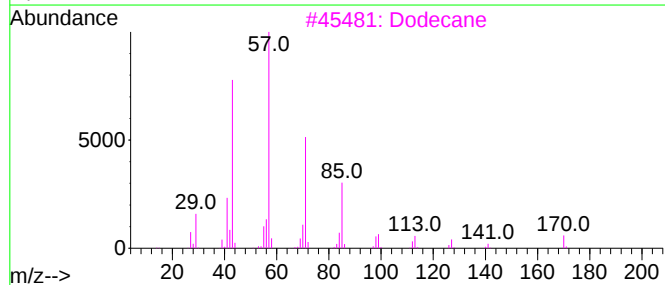
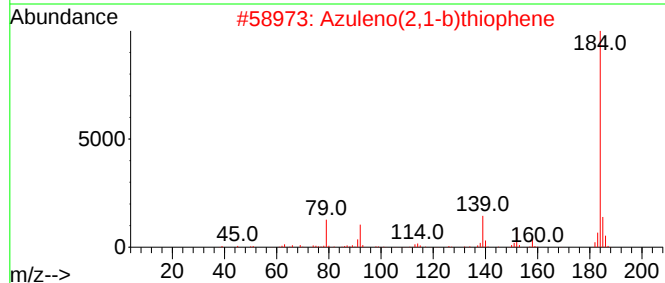
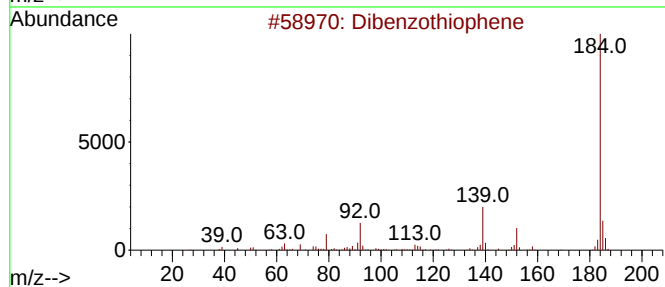
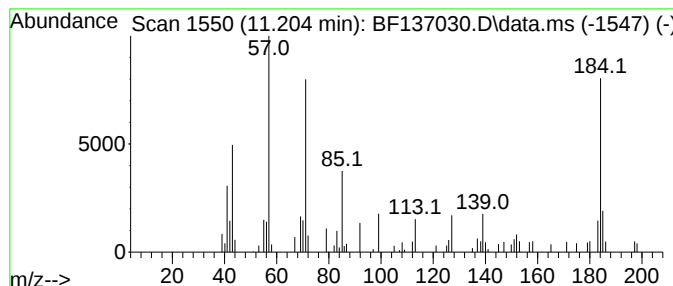
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown11.204 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	2.28 ng	37808	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzothiophene	184	C12H8S	000132-65-0	38
2			Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	38
3			Dodecane	170	C12H26	000112-40-3	35
4			5,5-Dibutylnonane	240	C17H36	006008-17-9	35
5			Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137030.D
Acq On : 10 Jan 2024 20:33
Operator : CG\JU
Sample : P1068-01
Misc :
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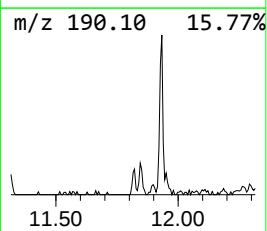
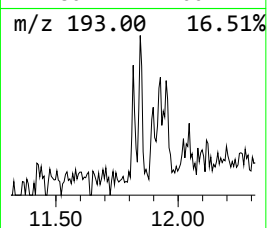
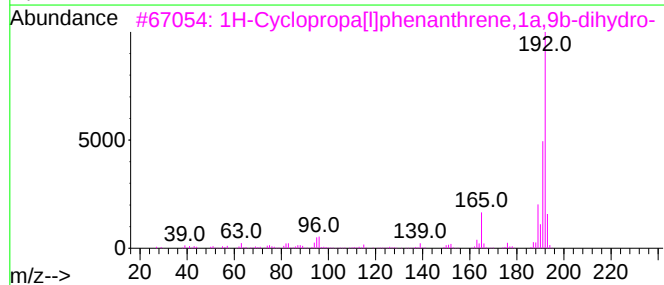
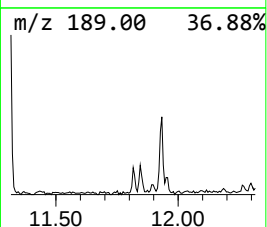
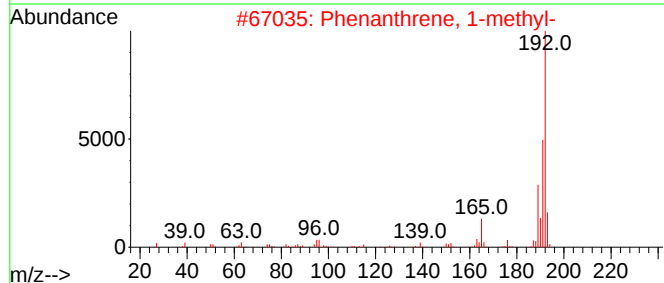
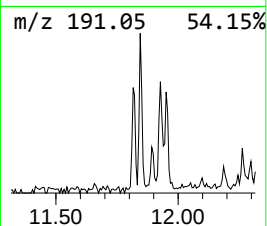
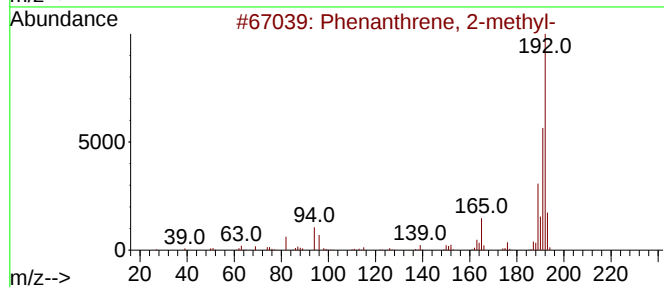
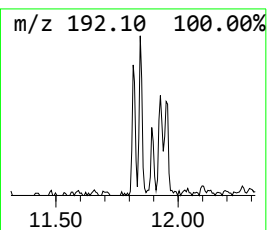
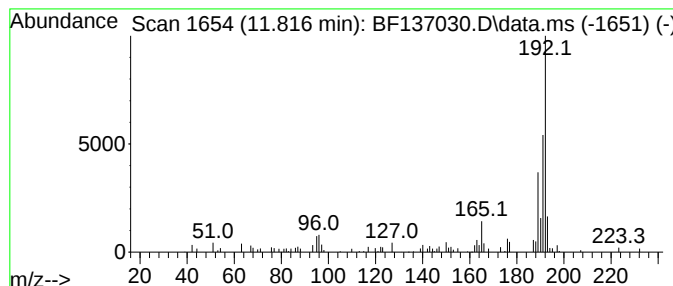
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	2.40 ng	39805	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3			1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137030.D
Acq On : 10 Jan 2024 20:33
Operator : CG\JU
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Instrument :
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ClientSampleId :
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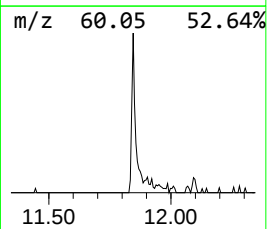
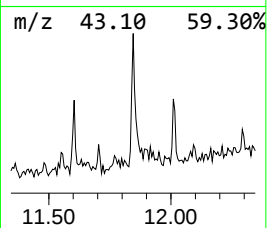
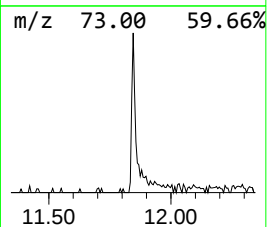
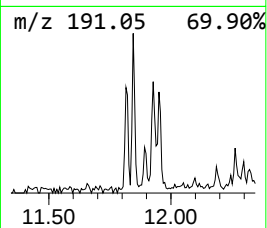
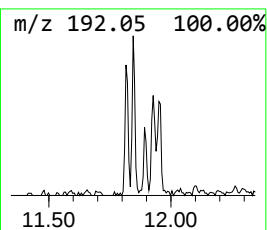
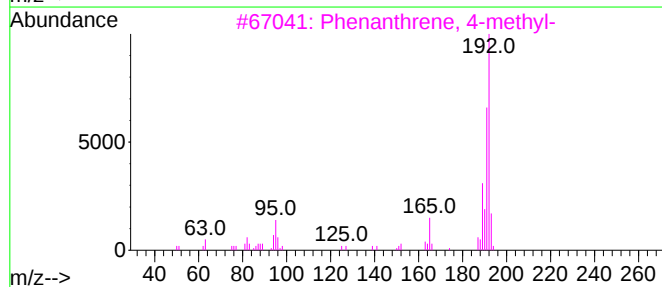
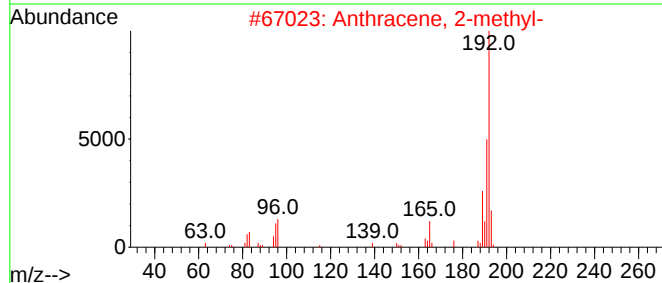
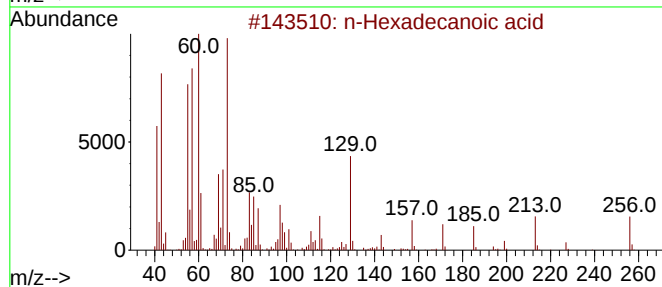
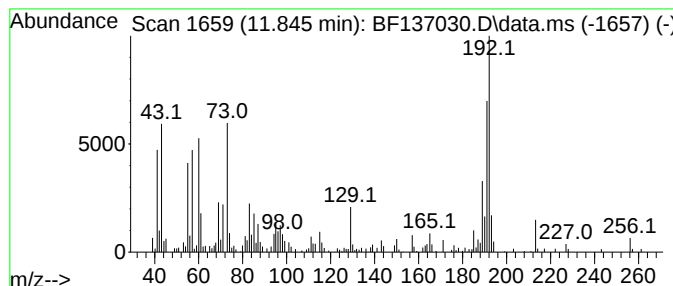
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	7.58 ng	125804	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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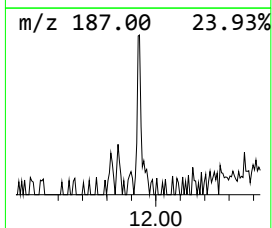
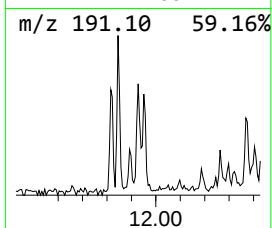
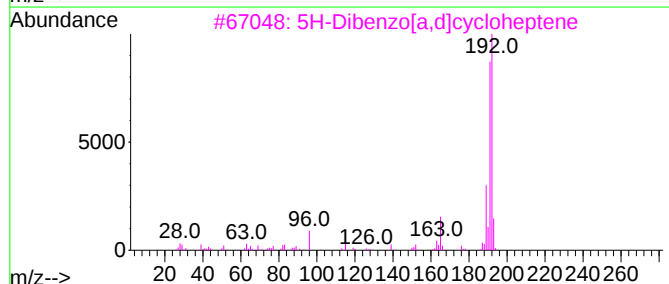
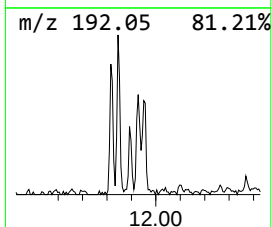
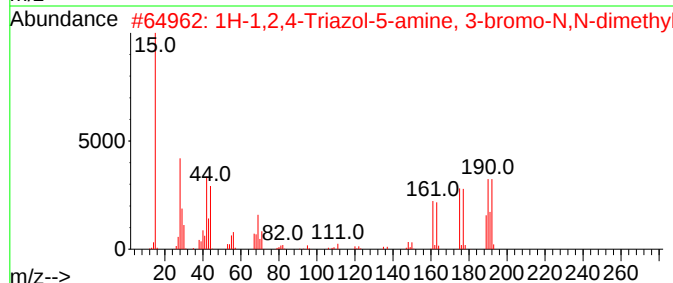
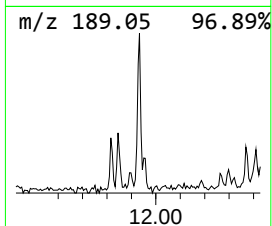
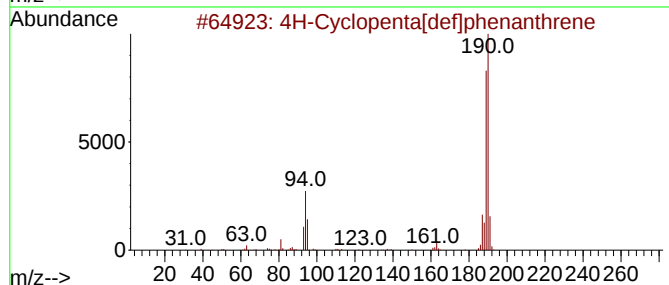
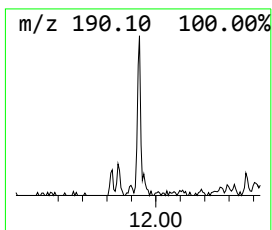
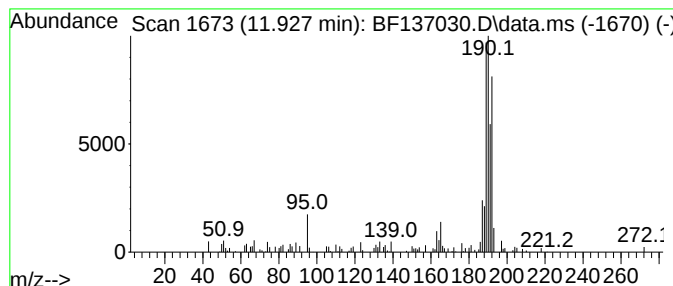
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.927	3.98 ng	66015	Phenanthrene-d10		11.316	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	60
2	1H-1,2,4-Triazol-5-amine, 3-brom...		190	C4H7BrN4	1000460-85-7	53
3	5H-Dibenzo[a,d]cycloheptene		192	C15H12	000256-81-5	38
4	Benzene, 1,1'-(2-cyclopropen-1-y...		192	C15H12	022825-21-4	35
5	Anthracene, 2-methyl-		192	C15H12	000613-12-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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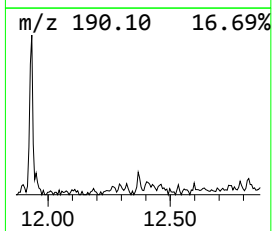
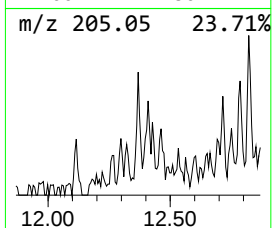
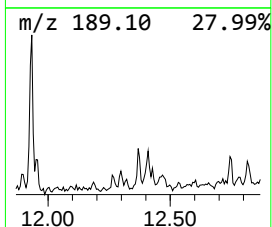
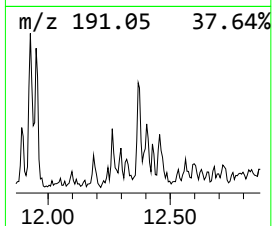
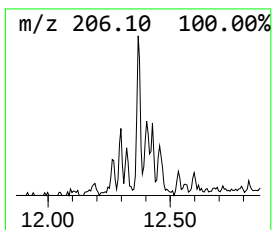
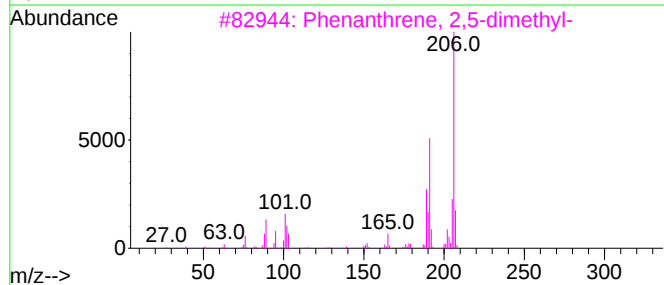
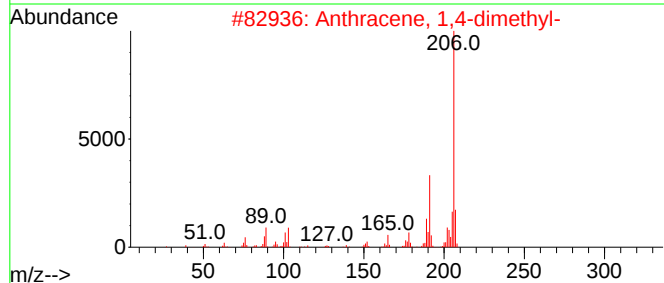
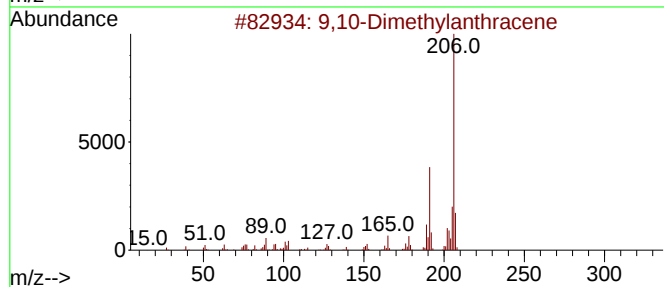
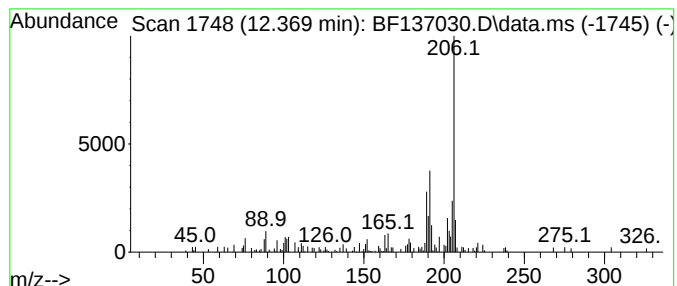
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9,10-Dimethylantracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.369	2.21 ng	36768	Phenanthrene-d10		11.316	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylantracene		206	C16H14	000781-43-1	96
2	Anthracene, 1,4-dimethyl-		206	C16H14	000781-92-0	94
3	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	93
4	Phenanthrene, 3,6-dimethyl-		206	C16H14	001576-67-6	93
5	Phenanthrene, 1,7-dimethyl-		206	C16H14	000483-87-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137030.D
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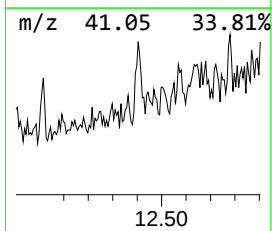
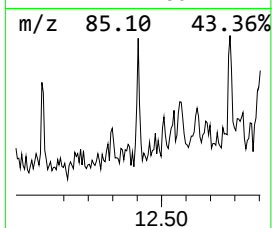
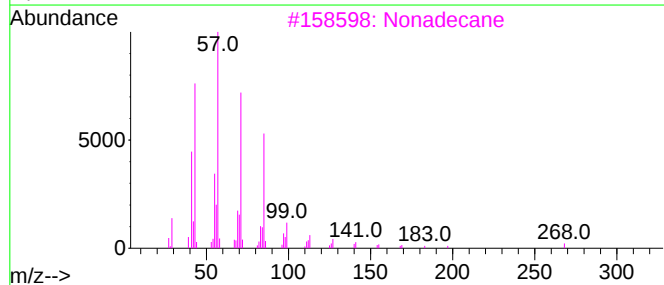
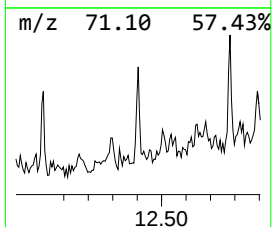
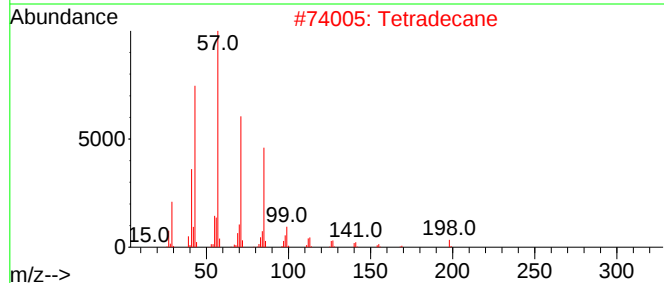
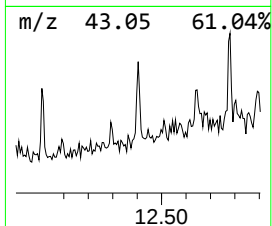
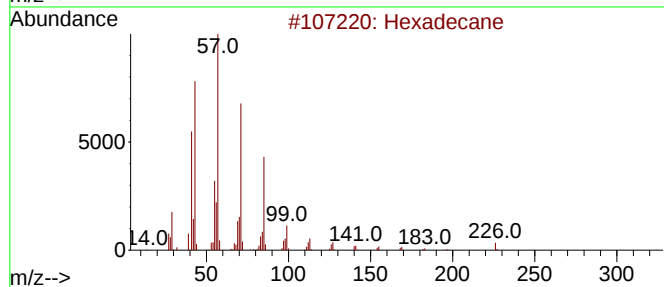
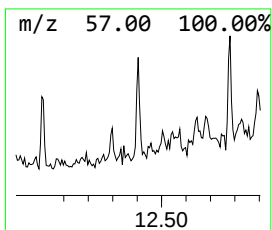
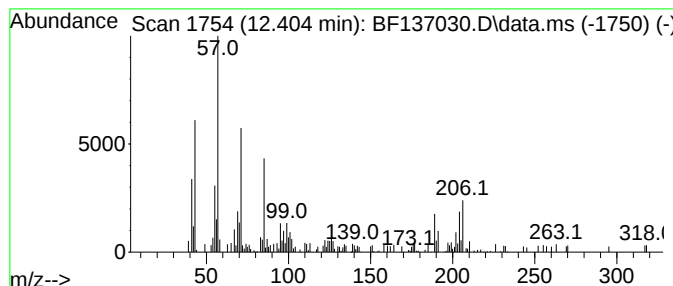
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	5.12 ng	84971	Phenanthrene-d10	11.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	86
2		Tetradecane	198	C14H30	000629-59-4	64
3		Nonadecane	268	C19H40	000629-92-5	45
4		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	45
5		Eicosane	282	C20H42	000112-95-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137030.D
Acq On : 10 Jan 2024 20:33
Operator : CG\JU
Sample : P1068-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-010824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-Pentanone, 4-...	5.016	4.5	ng	57626	1	6.787	258353	20.0
Dodecane, 2,6,1...	9.216	2.3	ng	34627	3	9.816	304248	20.0
Naphthalene, 1,...	9.475	2.1	ng	32220	3	9.816	304248	20.0
Heptadecane, 7-...	10.733	3.5	ng	58093	4	11.316	332124	20.0
unknown11.204	11.204	2.3	ng	37808	4	11.316	332124	20.0
Phenanthrene, 2...	11.816	2.4	ng	39805	4	11.316	332124	20.0
n-Hexadecanoic ...	11.845	7.6	ng	125804	4	11.316	332124	20.0
4H-Cyclopenta[d...]	11.927	4.0	ng	66015	4	11.316	332124	20.0
9,10-Dimethylan...	12.369	2.2	ng	36768	4	11.316	332124	20.0
Hexadecane	12.404	5.1	ng	84971	4	11.316	332124	20.0