

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
 Data File : BF139098.D
 Acq On : 21 Aug 2024 13:21
 Operator : RC/JU
 Sample : P3660-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-906-J-0-0.5-081624

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-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	19	26	rVB	1156050	1785226	92.44%	10.057%
2	2.310	31	37	45	rVB	14473	22599	1.17%	0.127%
3	3.399	216	222	237	rBV	40158	94776	4.91%	0.534%
4	3.993	317	323	329	rBV	20021	30259	1.57%	0.170%
5	5.116	504	514	520	rBV	83666	131197	6.79%	0.739%
6	5.510	575	581	586	rBV	1430603	1854239	96.01%	10.446%
7	6.181	690	695	702	rVB	38689	48975	2.54%	0.276%
8	6.445	736	740	745	rBV2	36237	45358	2.35%	0.256%
9	6.516	745	752	757	rBV	1355016	1931211	100.00%	10.880%
10	6.716	781	786	792	rBV	26700	32781	1.70%	0.185%
11	6.892	811	816	821	rBV	495615	621768	32.20%	3.503%
12	7.051	840	843	847	rVB	16693	19514	1.01%	0.110%
13	7.287	877	883	887	rBV	18062	23142	1.20%	0.130%
14	7.451	905	911	917	rBV	898737	1201379	62.21%	6.768%
15	7.710	950	955	959	rBV	17981	21572	1.12%	0.122%
16	7.857	972	980	986	rVB	28514	39578	2.05%	0.223%
17	8.175	1029	1034	1041	rBV	645435	815896	42.25%	4.597%
18	8.392	1065	1071	1077	rVB2	19400	25586	1.32%	0.144%
19	8.486	1082	1087	1096	rVV	71509	93498	4.84%	0.527%
20	8.863	1144	1151	1157	rBV	25128	32788	1.70%	0.185%
21	9.033	1175	1180	1184	rBV	46582	58487	3.03%	0.329%
22	9.251	1211	1217	1222	rBV	1364448	1662399	86.08%	9.365%
23	9.345	1222	1233	1238	rBV2	26405	46260	2.40%	0.261%
24	9.928	1327	1332	1337	rBV	708651	883088	45.73%	4.975%
25	10.028	1343	1349	1356	rBV	40864	61909	3.21%	0.349%
26	10.716	1461	1466	1471	rBV	936305	1172542	60.72%	6.606%
27	11.416	1580	1585	1593	rBV2	636098	873345	45.22%	4.920%
28	11.945	1665	1675	1680	rBV	112388	174555	9.04%	0.983%
29	12.027	1685	1689	1698	rVB	15469	29254	1.51%	0.165%
30	12.227	1716	1723	1728	rBV2	11096	20116	1.04%	0.113%
31	12.627	1785	1791	1803	rBV	146624	239008	12.38%	1.347%
32	12.727	1803	1808	1814	rBV	40147	56930	2.95%	0.321%
33	12.851	1821	1829	1835	rBV	116216	179627	9.30%	1.012%
34	12.998	1849	1854	1859	rVB	766098	954625	49.43%	5.378%
35	13.180	1876	1885	1888	rBV3	12403	24849	1.29%	0.140%
36	13.363	1912	1916	1921	rBV2	23752	32282	1.67%	0.182%

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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

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37	13.692	1967	1972	1979	rVB2	14597	27647	1.43%	0.156%
38	13.851	1993	1999	2003	rVV3	16441	30078	1.56%	0.169%
39	13.904	2003	2008	2016	rVB2	77139	117472	6.08%	0.662%
40	14.051	2024	2033	2043	rBV2	449963	743430	38.50%	4.188%
41	14.433	2090	2098	2102	rBV2	9365	19786	1.02%	0.111%
42	14.533	2110	2115	2122	rBV3	44316	76903	3.98%	0.433%
43	15.092	2205	2210	2222	rVB	81294	195105	10.10%	1.099%
44	15.198	2222	2228	2238	rVB4	23387	48485	2.51%	0.273%
45	15.404	2257	2263	2268	rBV	49981	83893	4.34%	0.473%
46	15.462	2268	2273	2278	rVV	53169	77510	4.01%	0.437%
47	15.527	2278	2284	2293	rVV	372522	561366	29.07%	3.163%
48	16.033	2365	2370	2374	rVV	13134	21406	1.11%	0.121%
49	16.080	2374	2378	2387	rVB8	16809	35365	1.83%	0.199%
50	16.433	2433	2438	2453	rVB6	29726	66908	3.46%	0.377%
51	16.998	2528	2534	2540	rBV2	24841	53868	2.79%	0.303%
52	17.215	2559	2571	2583	rBV9	20208	72814	3.77%	0.410%
53	17.392	2596	2601	2605	rBV7	9946	20974	1.09%	0.118%
54	17.439	2605	2609	2618	rVB	18471	38577	2.00%	0.217%
55	17.633	2634	2642	2655	rBV4	43471	118052	6.11%	0.665%

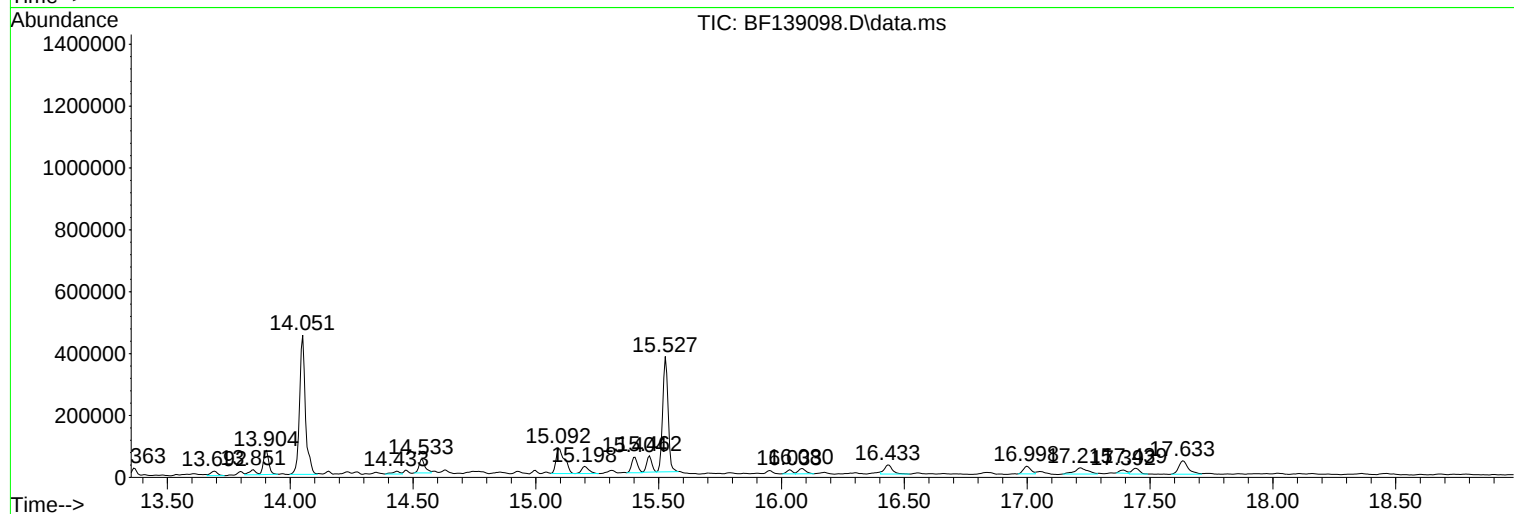
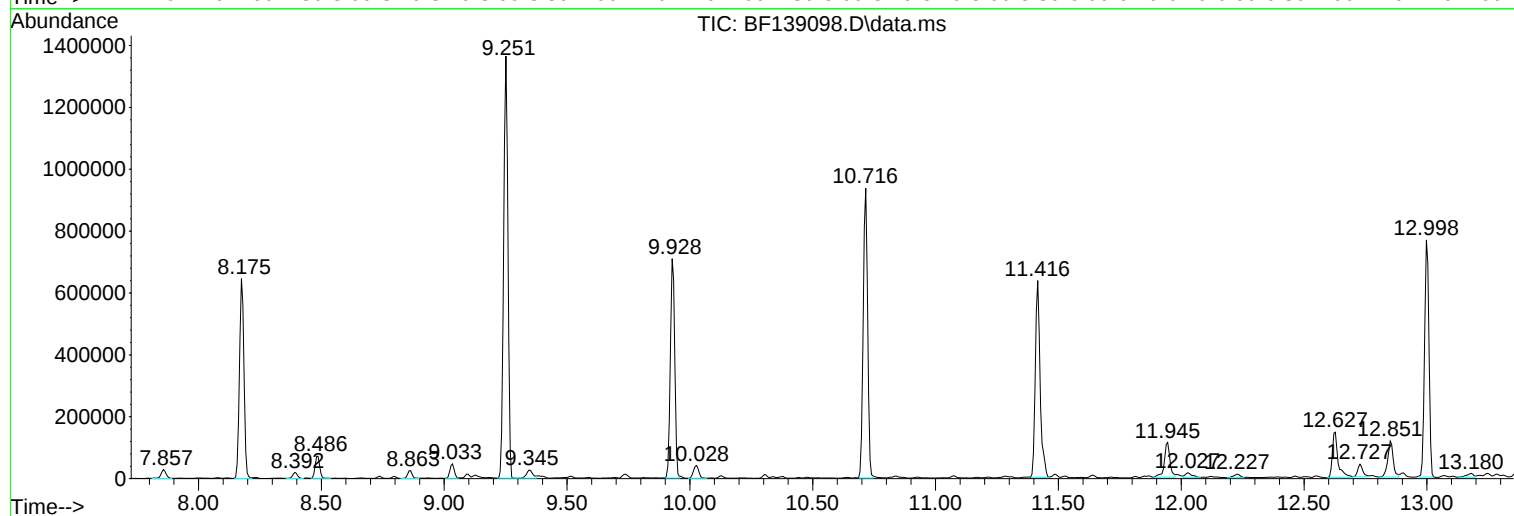
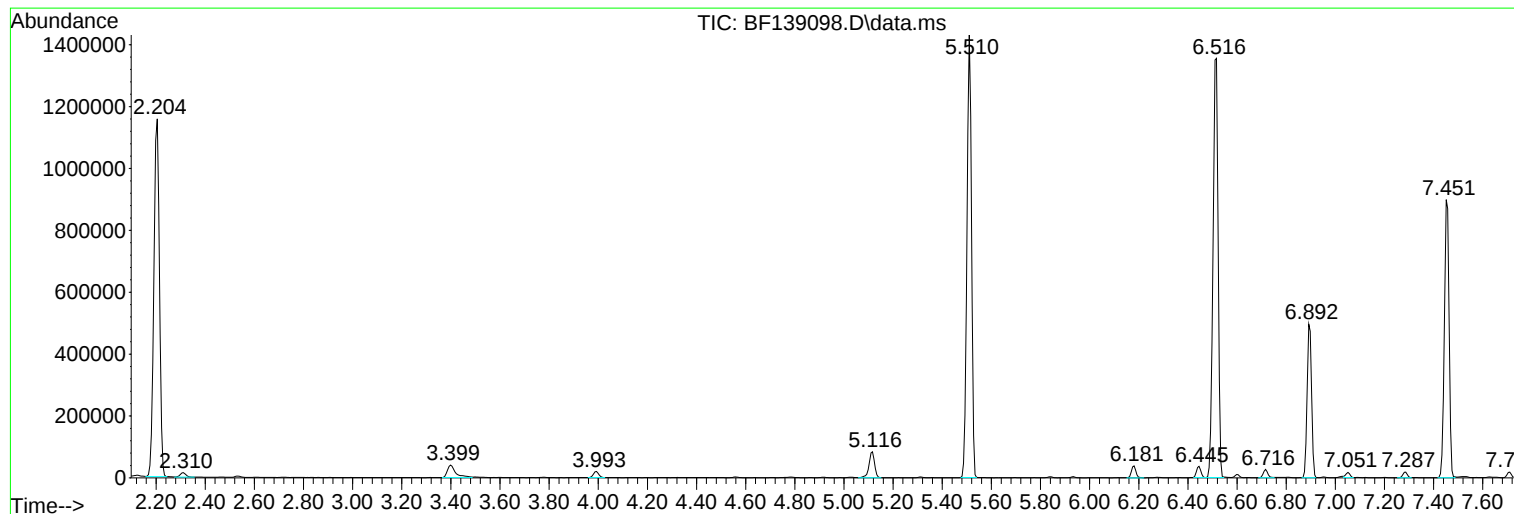
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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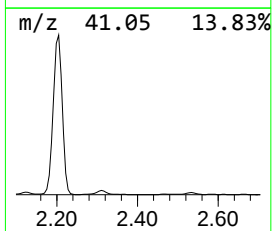
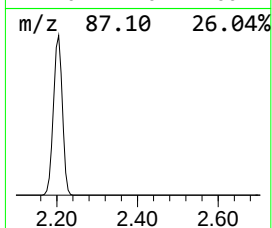
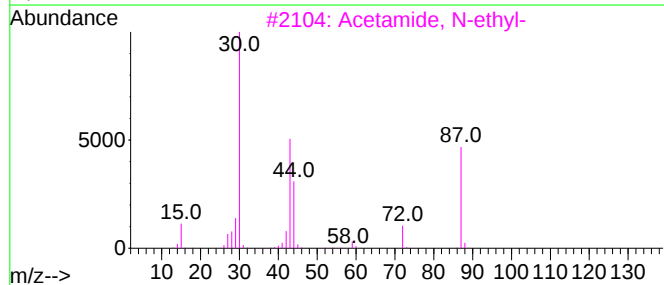
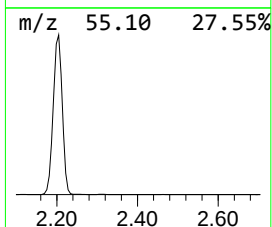
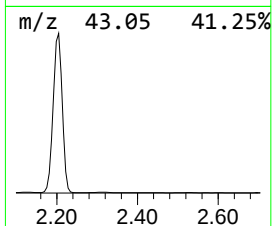
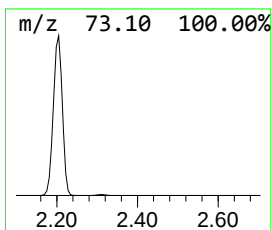
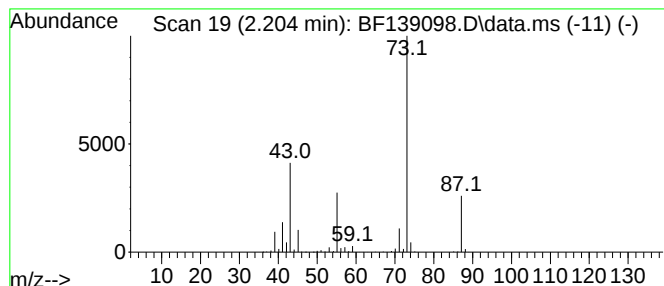
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	57.42 ng	1785230	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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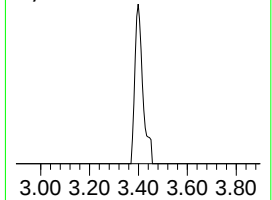
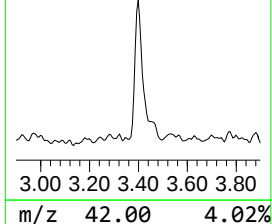
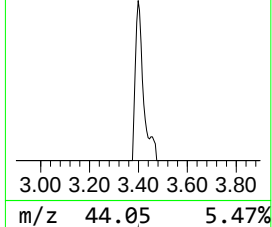
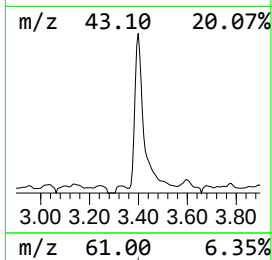
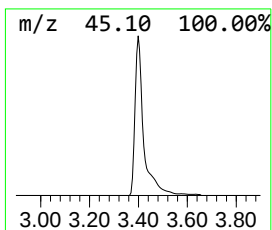
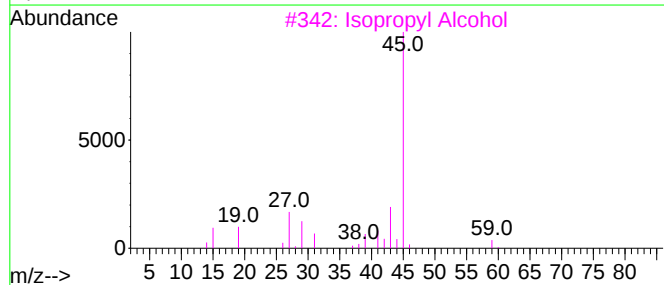
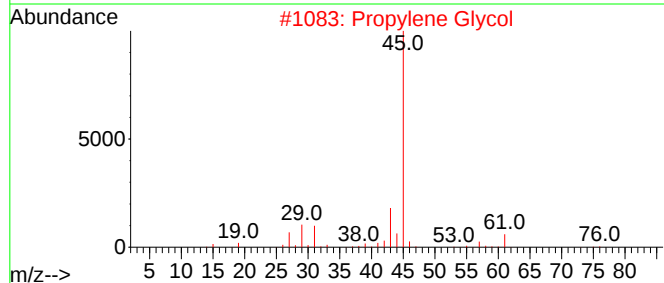
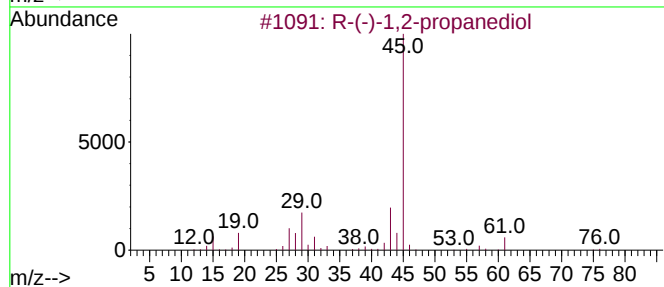
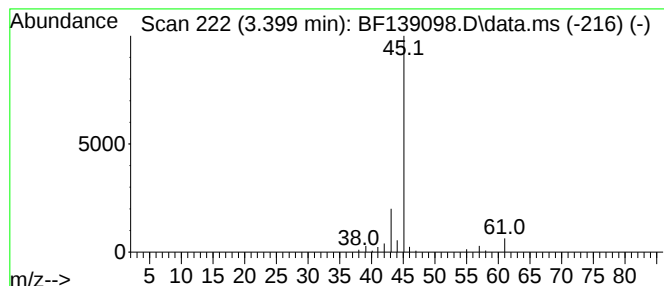
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	3.05 ng	94776	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	64
2	Propylene Glycol			76	C3H8O2	000057-55-6	43
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
4	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
5	Formamide			45	CH3NO	000075-12-7	5



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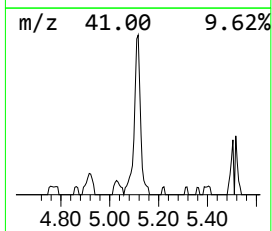
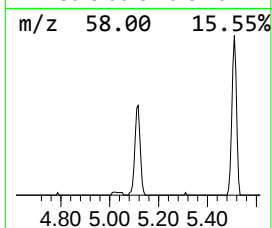
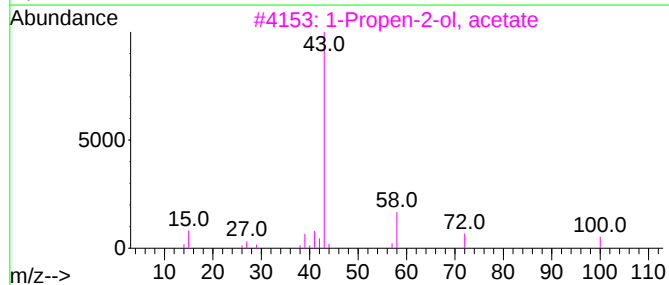
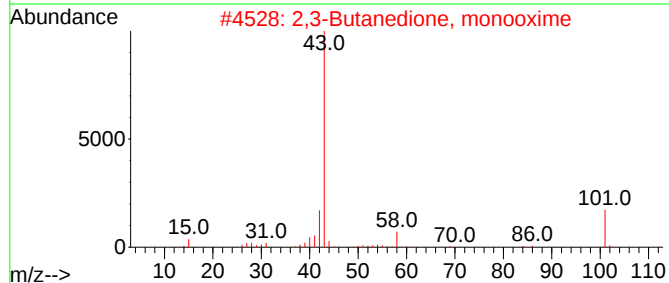
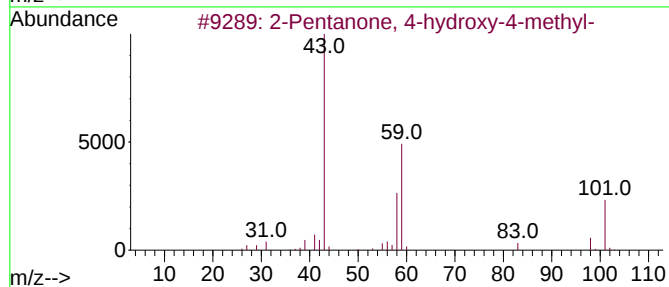
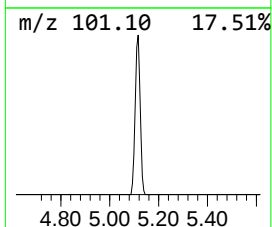
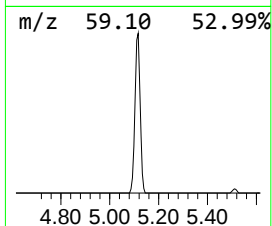
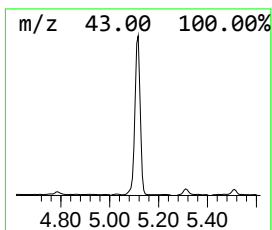
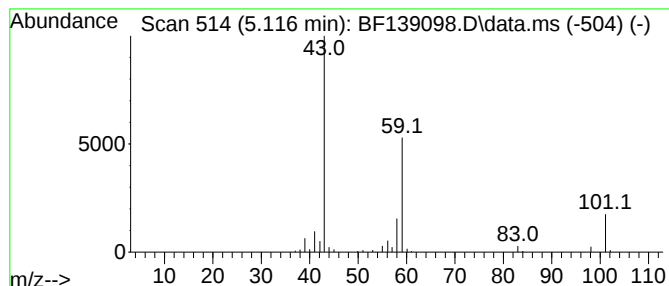
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	4.22 ng	131197	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Butane	58	C4H10	000106-97-8	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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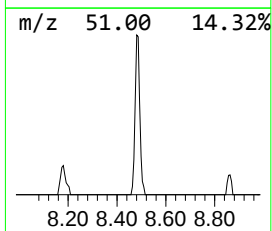
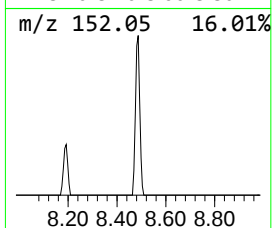
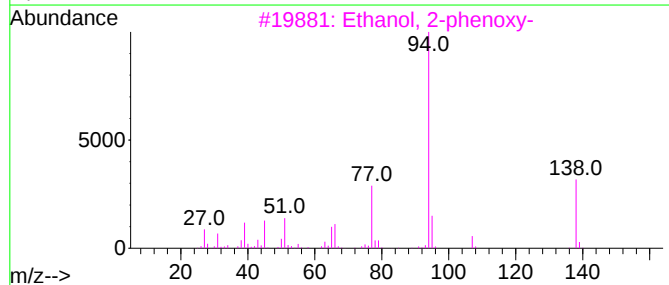
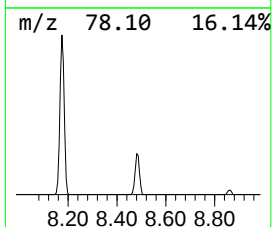
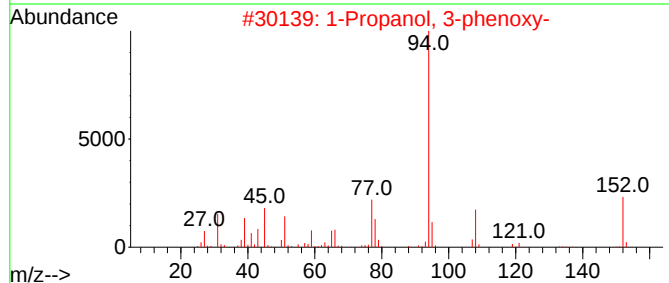
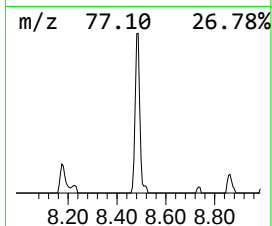
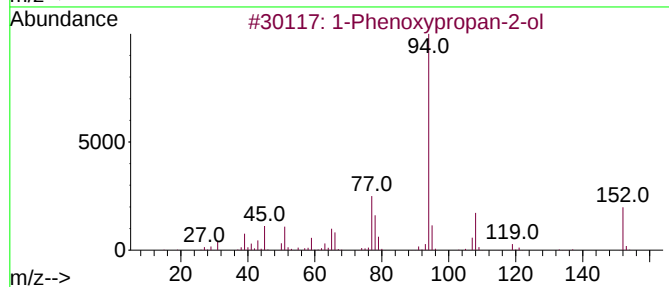
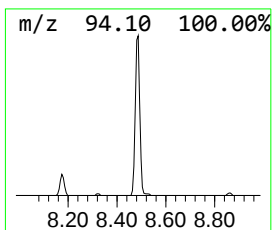
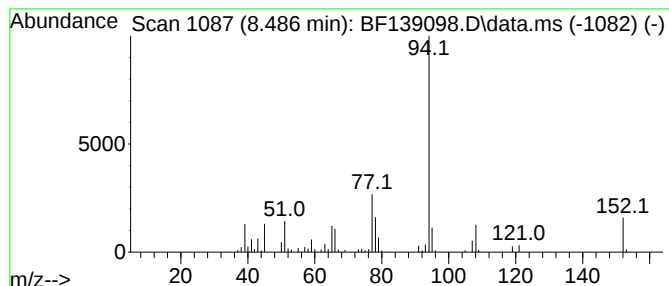
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	2.29 ng	93498	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53



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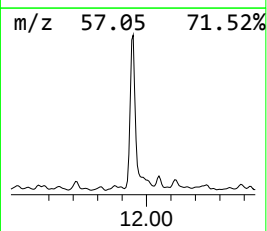
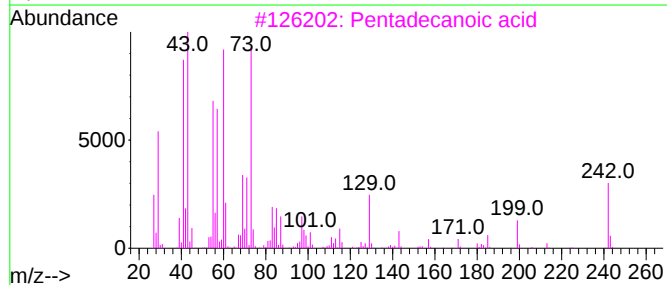
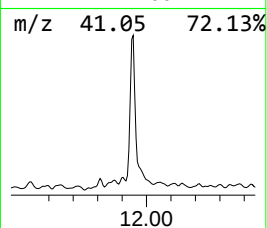
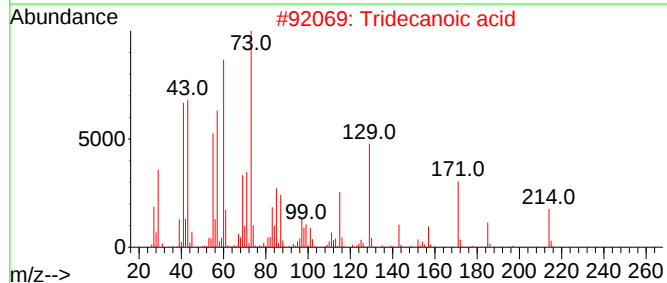
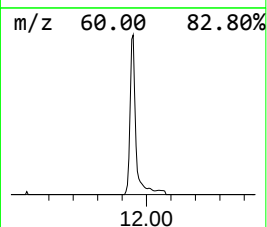
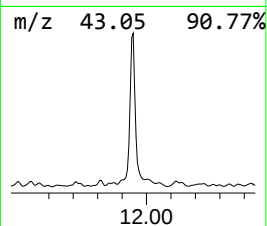
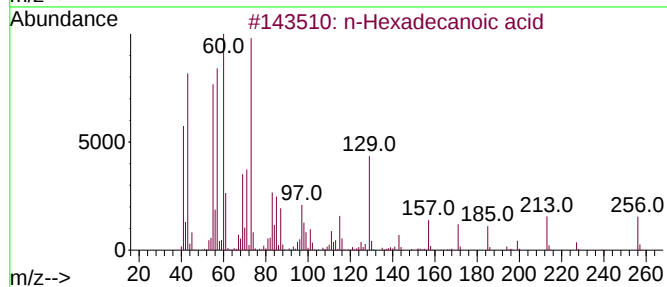
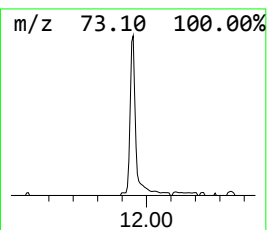
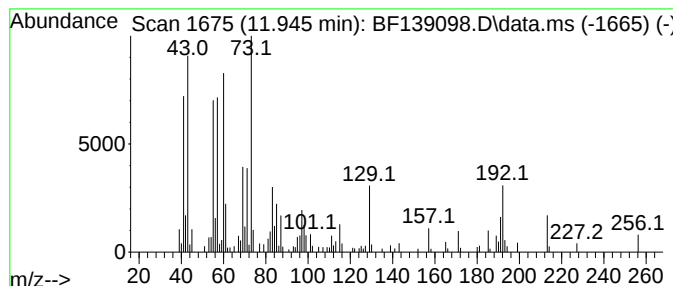
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	4.00 ng	174555	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

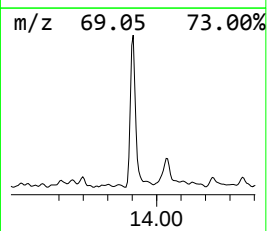
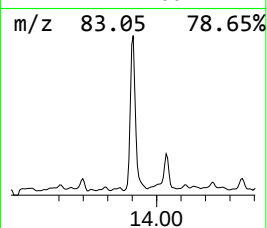
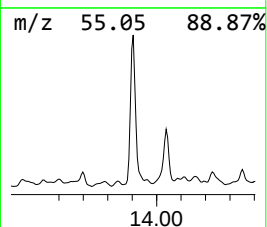
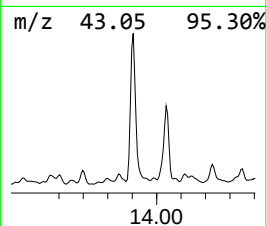
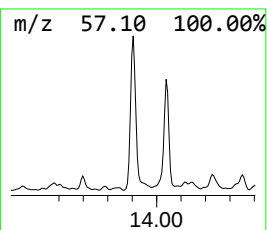
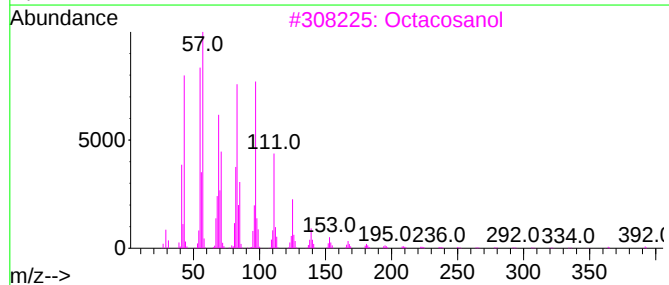
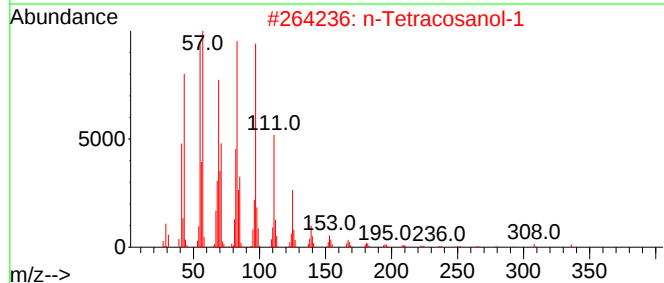
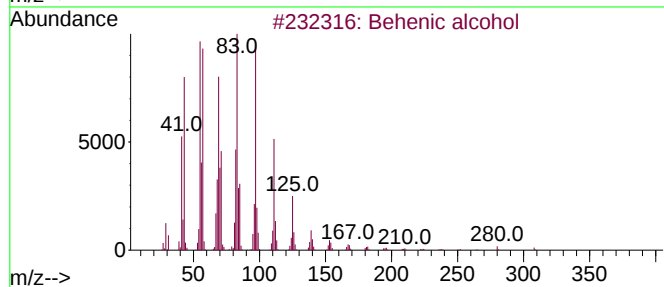
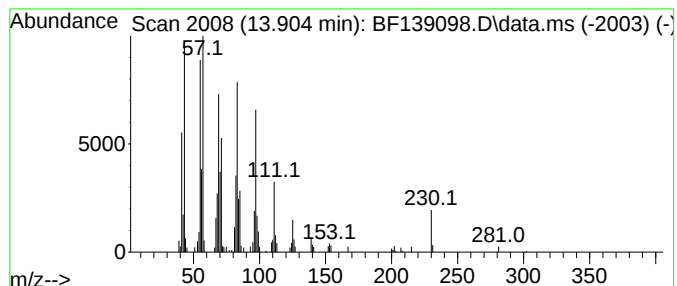
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.16 ng	117472	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3			Octacosanol	410	C28H58O	000557-61-9	93
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

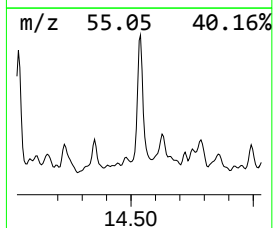
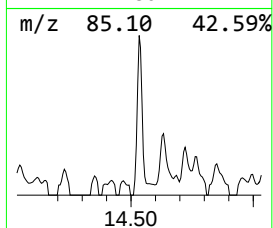
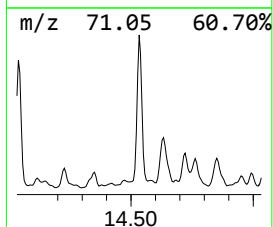
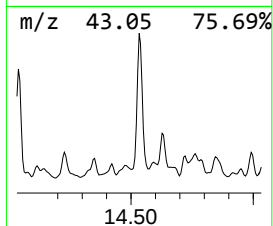
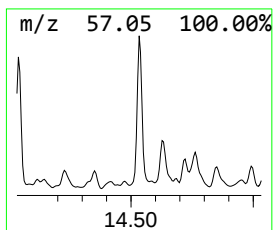
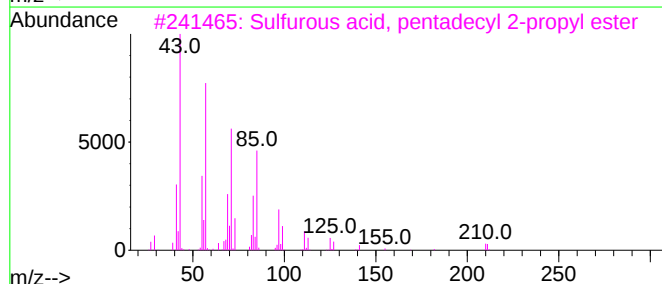
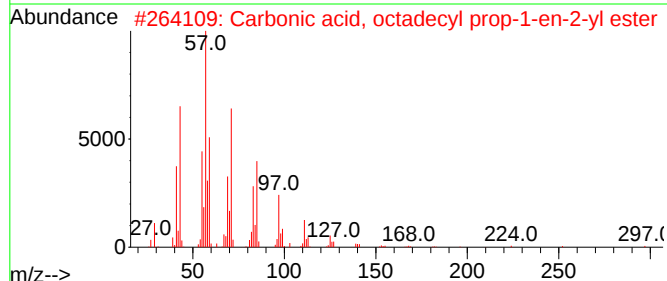
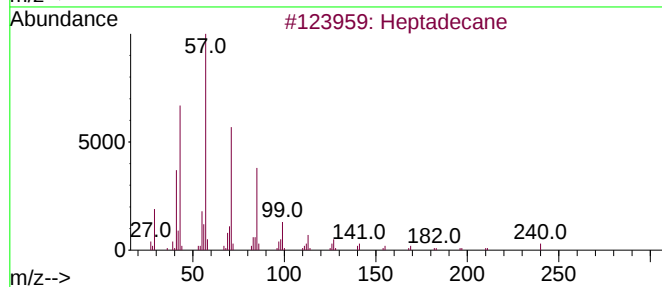
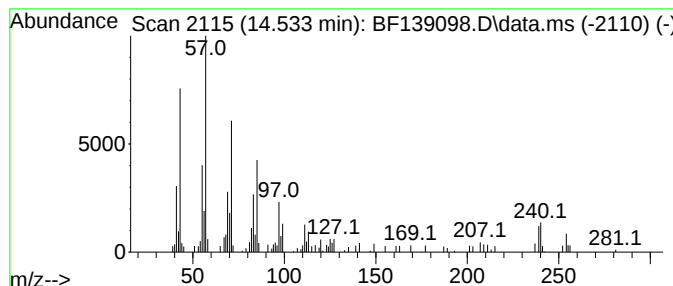
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.07 ng	76903	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	95
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	76
3			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	74
4			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	74
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

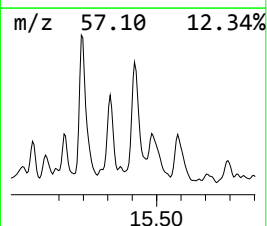
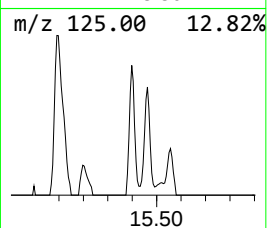
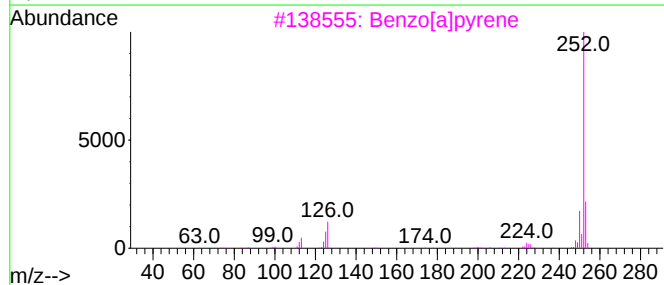
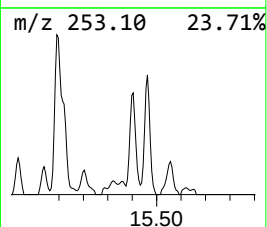
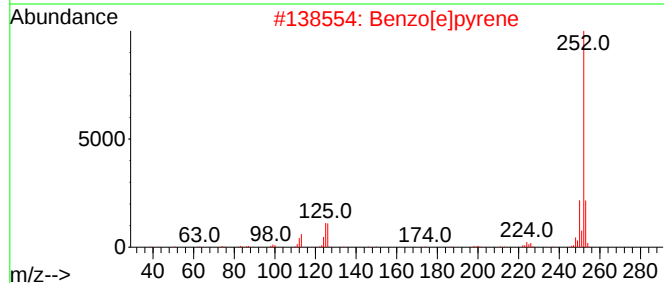
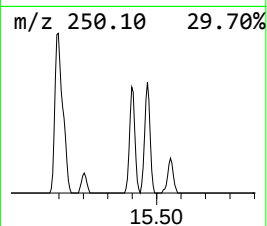
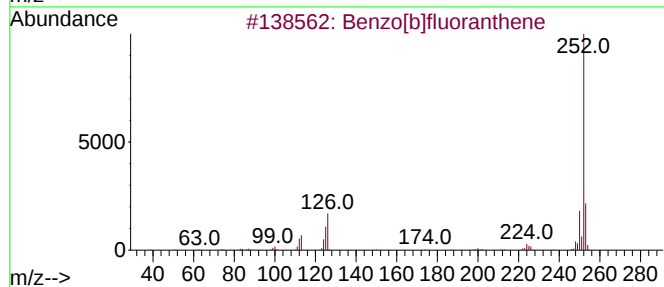
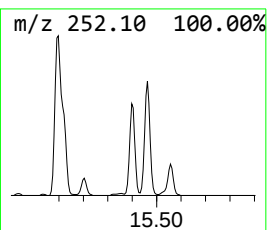
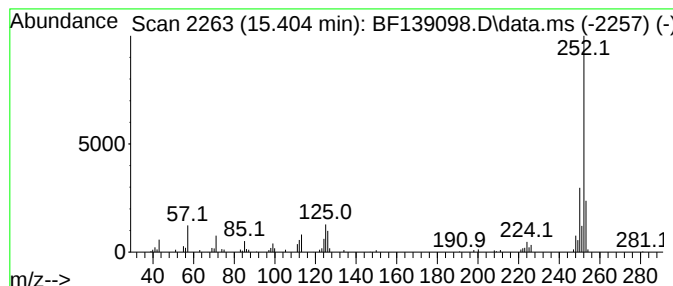
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.99 ng	83893	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Perylene	252	C20H12	000198-55-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

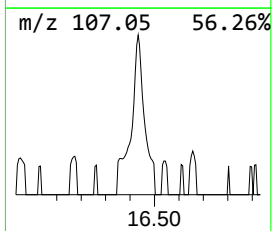
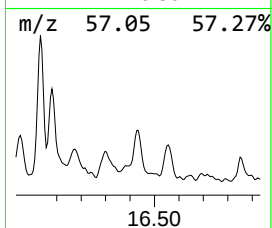
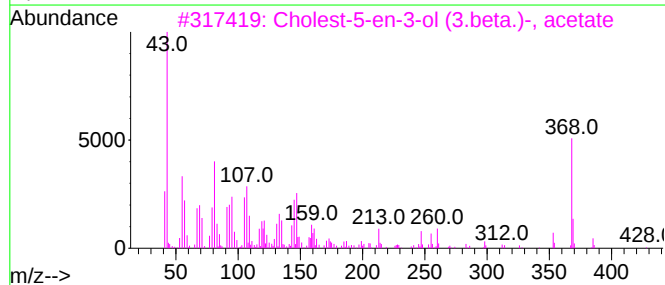
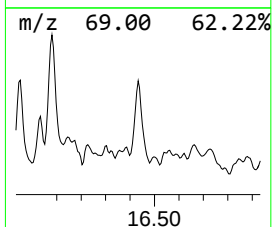
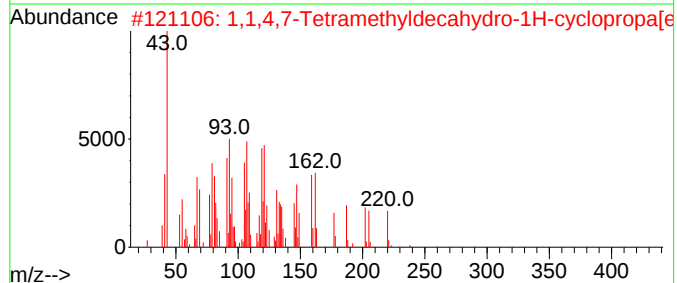
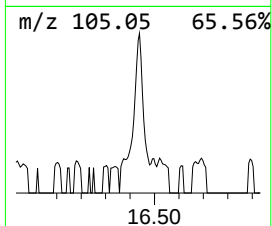
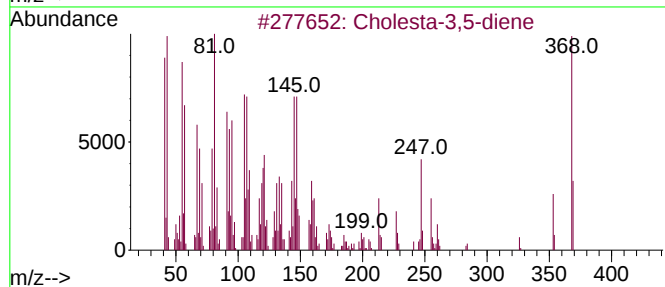
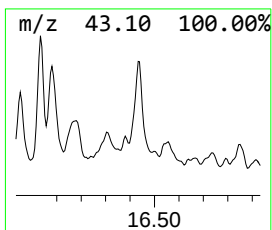
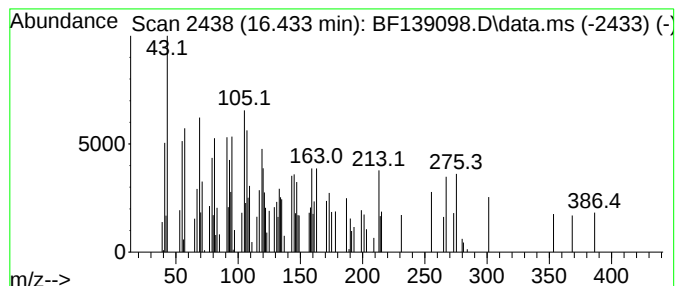
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.433 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.433	2.38 ng	66908	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholesta-3,5-diene	368	C27H44	000747-90-0	49
2			1,1,4,7-Tetramethyldecahydro-1H-...	238	C15H26O2	1212211-43-2	43
3			Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	27
4			Boscartol F	300	C20H28O2	1486443-17-7	27
5			Parthenolide	248	C15H20O3	020554-84-1	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

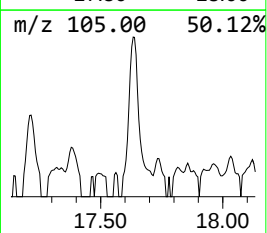
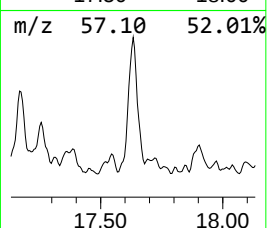
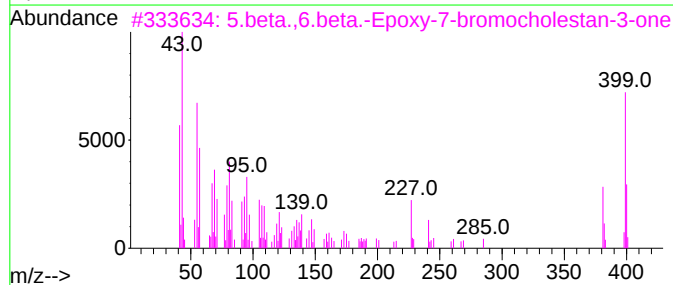
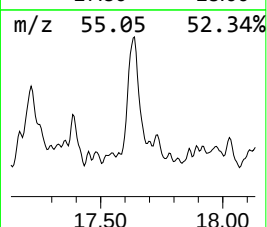
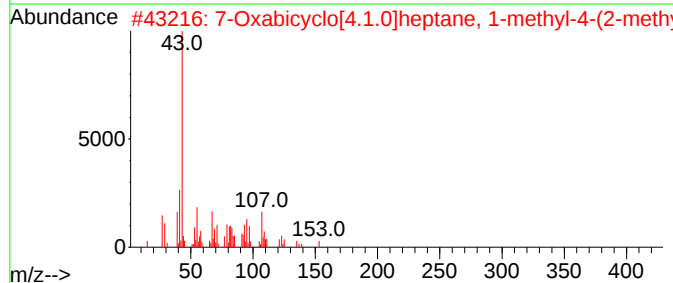
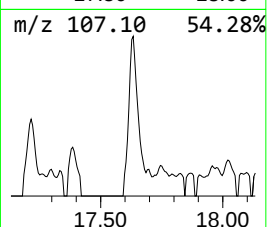
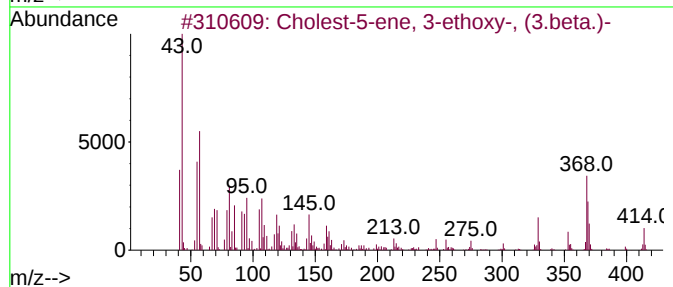
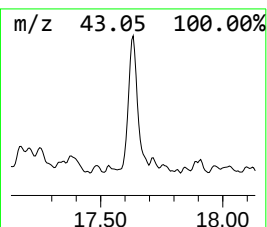
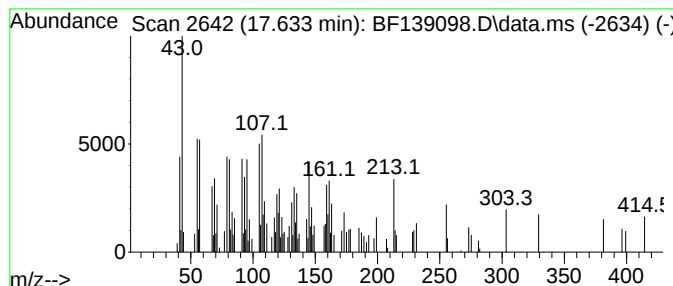
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.633 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.633	4.21 ng	118052	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	40
2			7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	27
3			5.beta.,6.beta.-Epoxy-7-bromocho...	478	C27H43BrO2	104825-82-3	16
4			Boscartol F	300	C20H28O2	1486443-17-7	14
5			Silane, chloroethenyldimethyl-	120	C4H9ClSi	001719-58-0	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139098.D
Acq On : 21 Aug 2024 13:21
Operator : RC/JU
Sample : P3660-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-906-J-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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
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R-(-)-1,2-propa...	3.399	3.0	ng	94776	1	6.892	621768	20.0
2-Pentanone, 4-...	5.116	4.2	ng	131197	1	6.892	621768	20.0
1-Phenoxypropan...	8.486	2.3	ng	93498	2	8.175	815896	20.0
n-Hexadecanoic ...	11.945	4.0	ng	174555	4	11.416	873345	20.0
Behenic alcohol	13.904	3.2	ng	117472	5	14.051	743430	20.0
Heptadecane	14.533	2.1	ng	76903	5	14.051	743430	20.0
Benzo[e]pyrene	15.404	3.0	ng	83893	6	15.527	561366	20.0
unknown16.433	16.433	2.4	ng	66908	6	15.527	561366	20.0
Naphthalene, 1,...	17.215	2.6	ng	72814	6	15.527	561366	20.0
unknown17.633	17.633	4.2	ng	118052	6	15.527	561366	20.0