

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
 Data File : BF134324.D
 Acq On : 17 Jul 2023 19:48
 Operator : CG\JU
 Sample : 03601-01RE
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-1-071223RE

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	499	507	513	rBV2	30537	54849	3.65%	0.483%
2	5.469	571	575	584	rBV	1456387	1353708	90.05%	11.916%
3	5.857	633	641	645	rVB4	13414	21832	1.45%	0.192%
4	6.087	674	680	682	rBV3	19904	26590	1.77%	0.234%
5	6.275	706	712	715	rBV3	16938	23075	1.53%	0.203%
6	6.363	724	727	735	rBV4	25211	34419	2.29%	0.303%
7	6.475	742	746	759	rBV	1370034	1358758	90.38%	11.960%
8	6.669	775	779	785	rBV2	52177	71033	4.73%	0.625%
9	6.840	804	808	813	rVB	447692	395606	26.32%	3.482%
10	7.104	847	853	856	rVB3	17202	19633	1.31%	0.173%
11	7.398	899	903	906	rBV	1013903	830848	55.27%	7.313%
12	7.475	911	916	919	rVB6	15072	19750	1.31%	0.174%
13	8.116	1022	1025	1028	rBV	587196	447923	29.80%	3.943%
14	8.528	1092	1095	1097	rBV	19391	19201	1.28%	0.169%
15	9.133	1195	1198	1204	rBV3	35371	36840	2.45%	0.324%
16	9.192	1204	1208	1211	rBV	1980561	1503309	100.00%	13.233%
17	9.269	1218	1221	1223	rBV3	25616	24705	1.64%	0.217%
18	9.304	1223	1227	1231	rVV2	29865	30462	2.03%	0.268%
19	9.586	1271	1275	1278	rVB3	26021	35629	2.37%	0.314%
20	9.733	1297	1300	1303	rBV2	21495	20813	1.38%	0.183%
21	9.869	1320	1323	1327	rVB	485169	440215	29.28%	3.875%
22	9.975	1337	1341	1345	rBV5	15561	19531	1.30%	0.172%
23	10.075	1356	1358	1363	rVB4	20478	22662	1.51%	0.199%
24	10.422	1414	1417	1423	rVB2	21434	28014	1.86%	0.247%
25	10.522	1430	1434	1439	rVB2	17879	26882	1.79%	0.237%
26	10.669	1455	1459	1462	rBV	911212	856573	56.98%	7.540%
27	10.786	1475	1479	1482	rBV	40014	46402	3.09%	0.408%
28	11.257	1556	1559	1565	rVB3	30408	39463	2.63%	0.347%
29	11.369	1574	1578	1580	rBV	507857	452813	30.12%	3.986%
30	11.392	1580	1582	1585	rVV	169523	129984	8.65%	1.144%
31	11.445	1588	1591	1593	rVB	32392	28368	1.89%	0.250%
32	11.875	1660	1664	1665	rBV	28091	32496	2.16%	0.286%
33	11.898	1665	1668	1675	rVB2	323171	304146	20.23%	2.677%
34	11.980	1680	1682	1685	rBV2	43896	42517	2.83%	0.374%
35	12.586	1782	1785	1788	rBV	249402	248499	16.53%	2.187%
36	12.686	1799	1802	1806	rBV	102249	114470	7.61%	1.008%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.821	1819	1825	1830	rBV	229681	260459	17.33%	2.293%
38	12.963	1845	1849	1853	rBV	1500769	1300635	86.52%	11.449%
39	14.027	2026	2030	2033	rBV2	327727	374143	24.89%	3.293%
40	15.539	2284	2287	2296	rVB	197316	263321	17.52%	2.318%

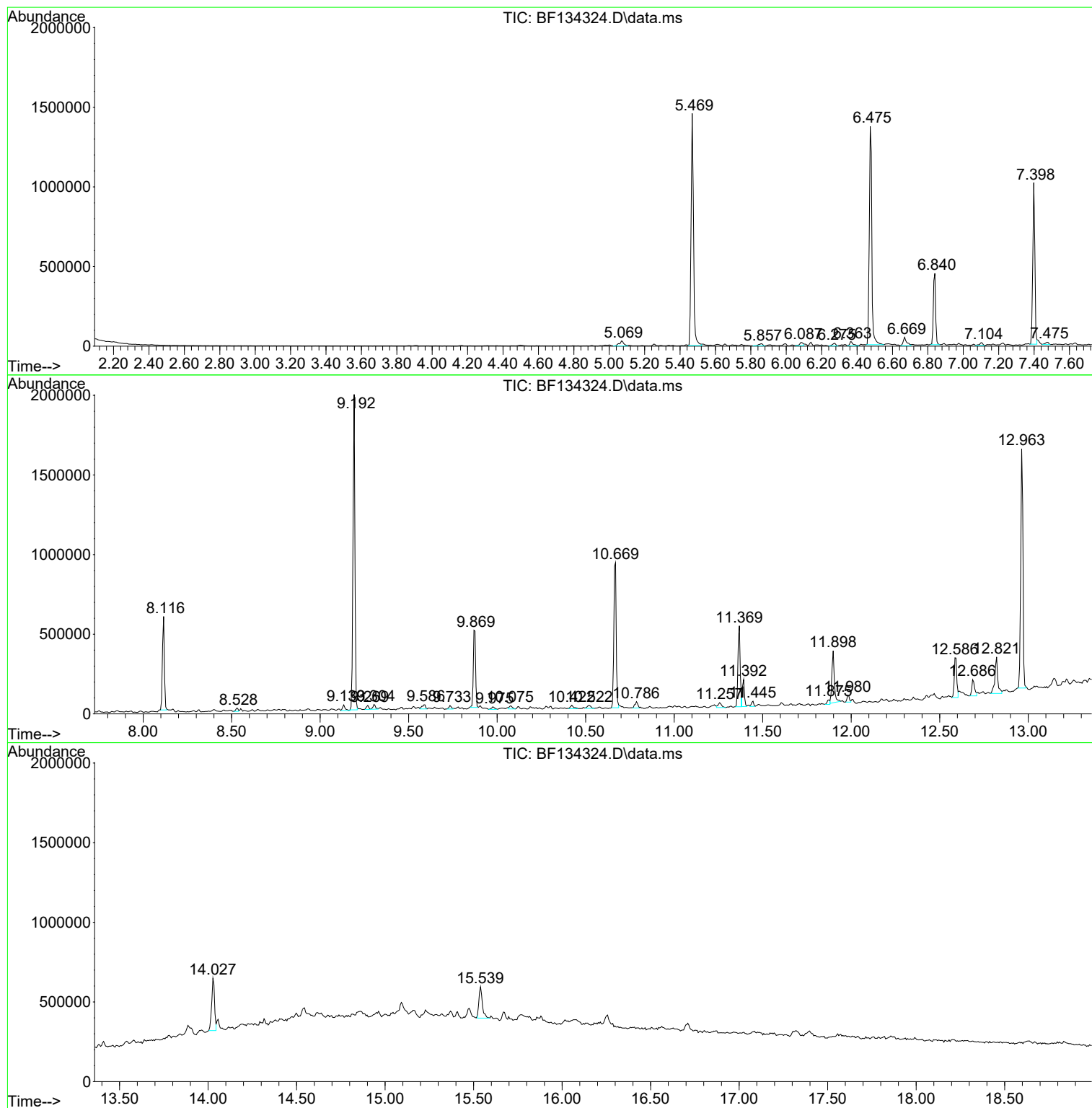
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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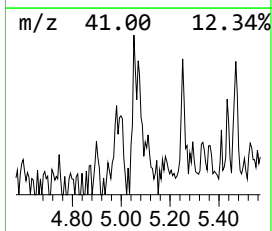
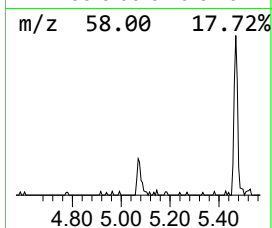
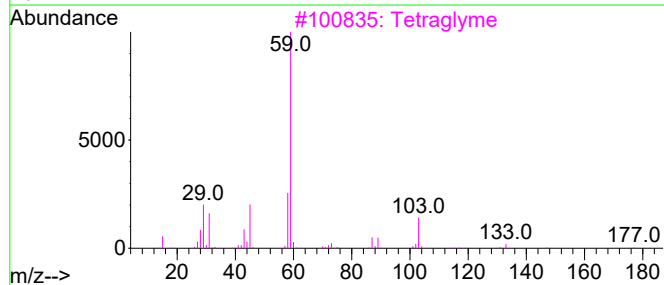
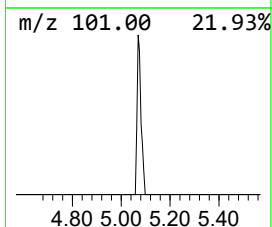
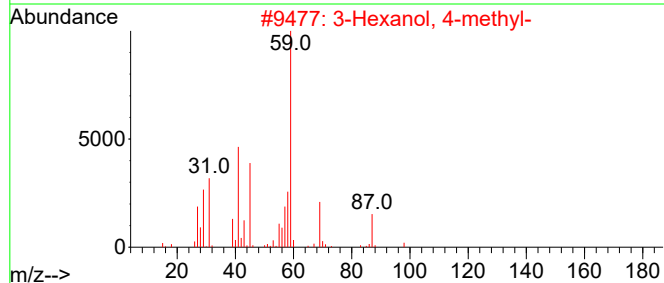
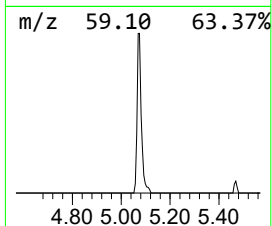
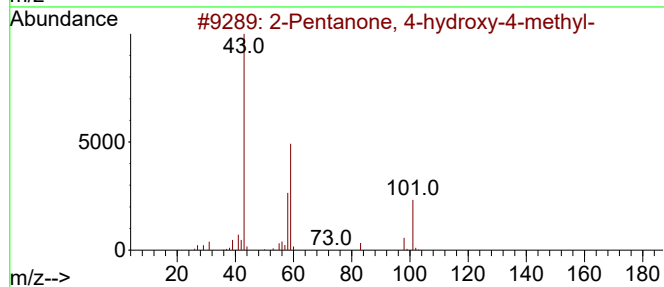
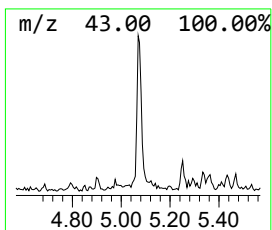
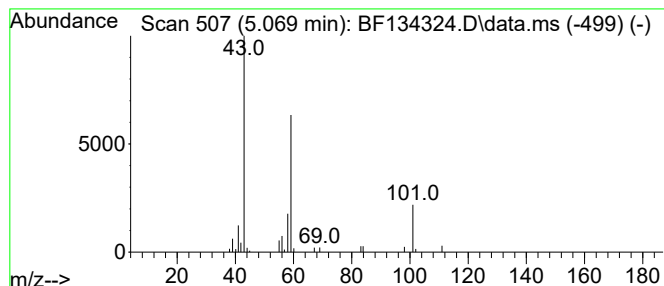
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.77 ng	54849	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
3	Tetraglyme	222	C10H22O5	000143-24-8	23		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	12		



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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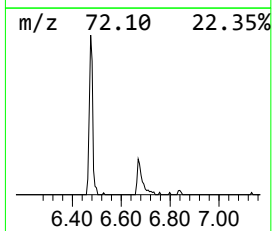
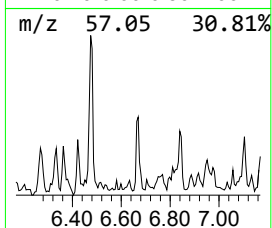
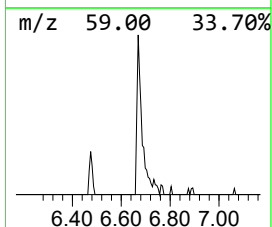
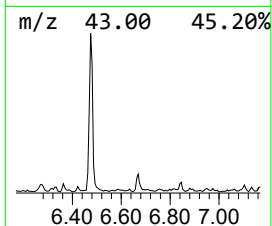
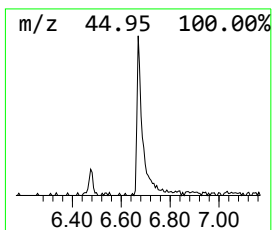
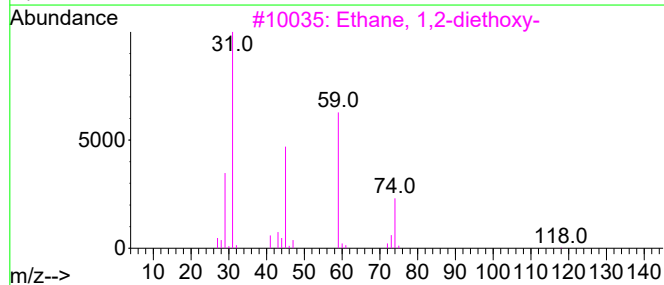
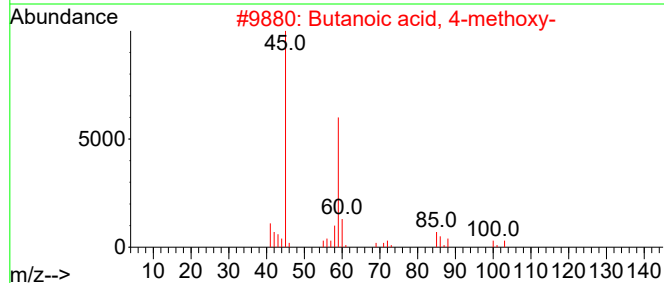
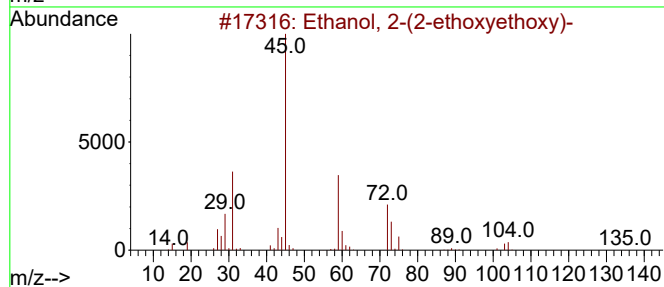
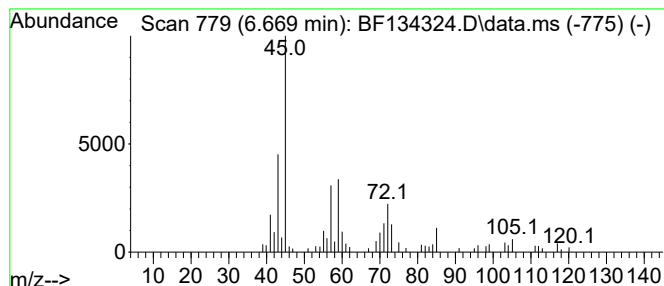
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.669	3.59 ng	71033	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	72
2			Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	53
3			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	47
4			Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	43
5			2-Octanol	130	C8H18O	000123-96-6	38



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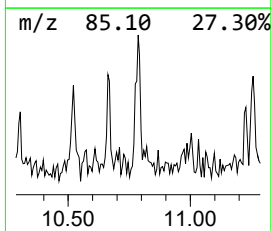
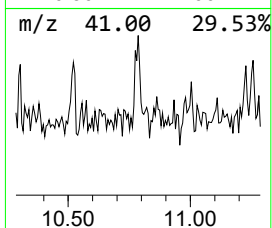
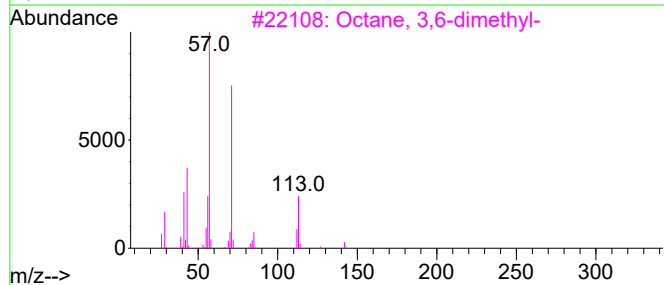
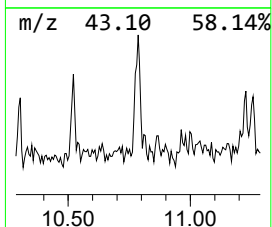
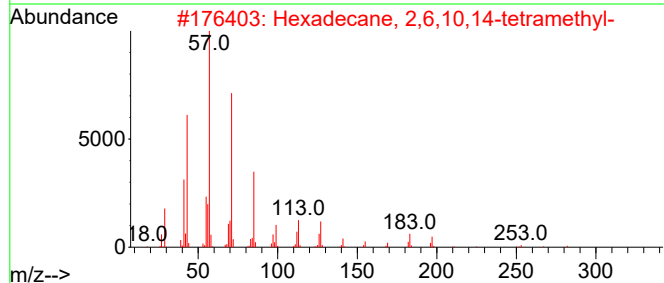
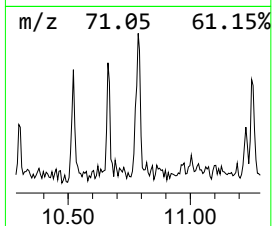
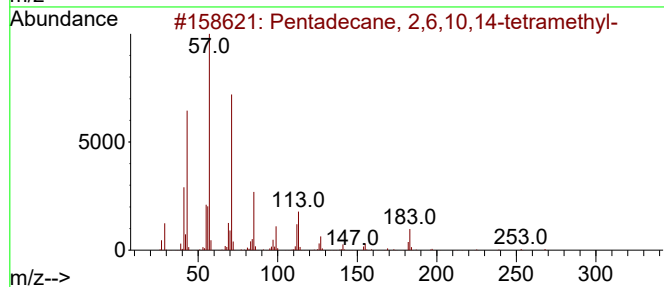
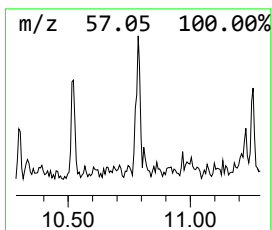
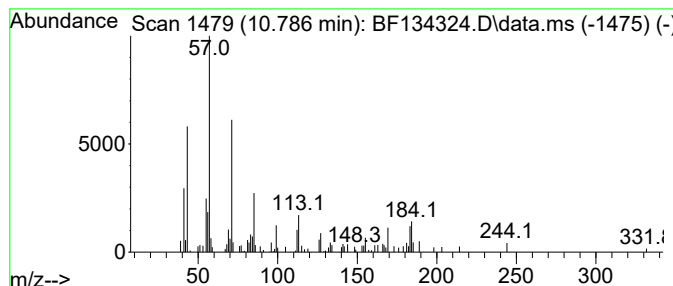
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecane, 2,6,10,14-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.786	2.05 ng	46402	Phenanthrene-d10			11.369
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-		268	C19H40	001921-70-6	74
2	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	64
3	Octane, 3,6-dimethyl-		142	C10H22	015869-94-0	55
4	Tridecane		184	C13H28	000629-50-5	52
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	52



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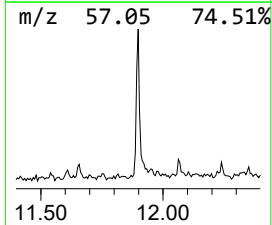
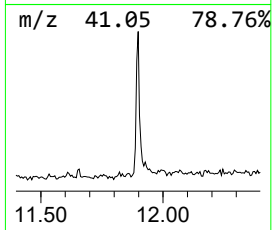
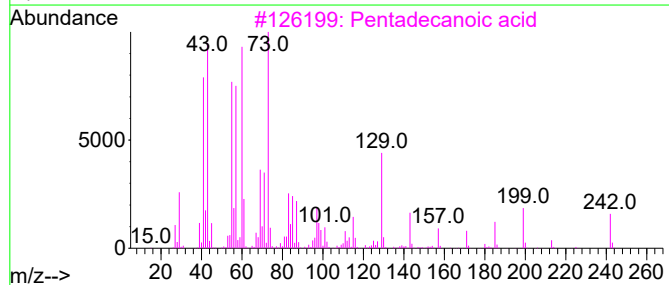
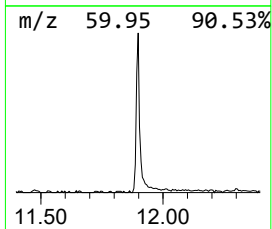
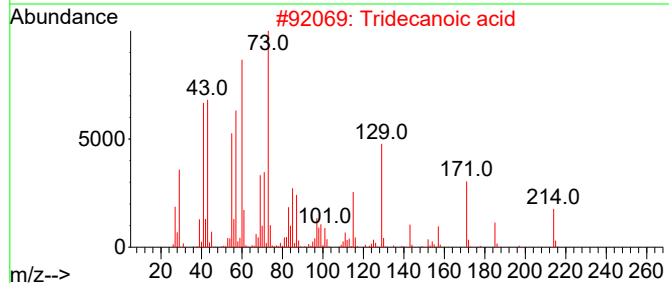
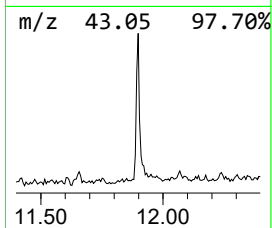
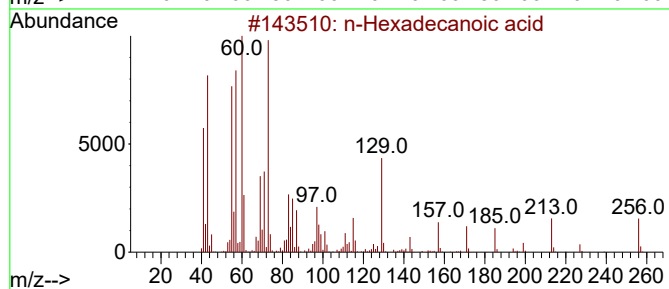
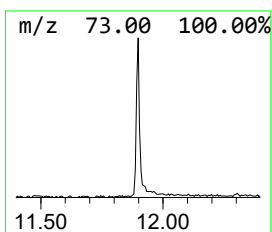
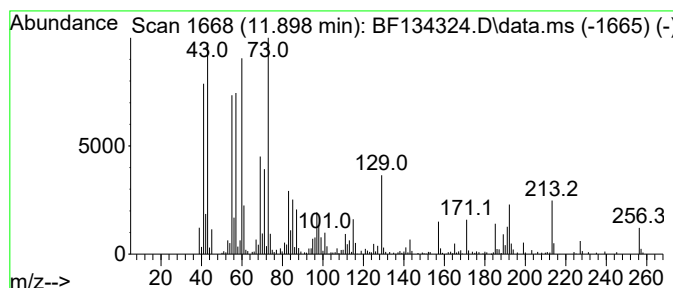
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	13.43 ng	304146	Phenanthrene-d10	11.369

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Undecanoic acid	186	C11H22O2	000112-37-8	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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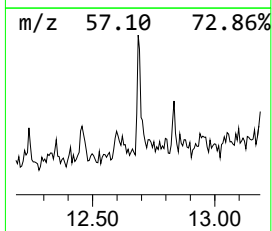
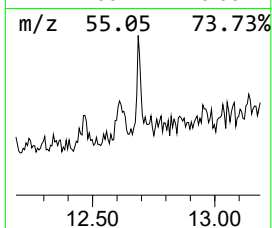
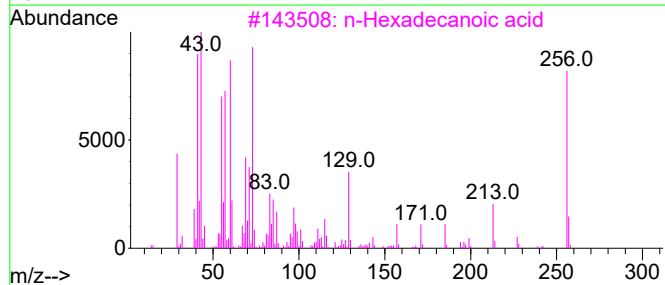
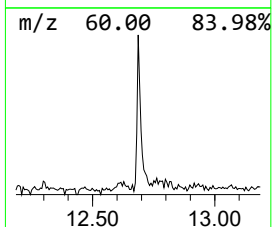
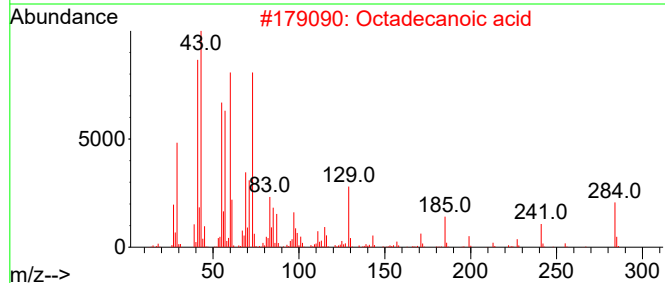
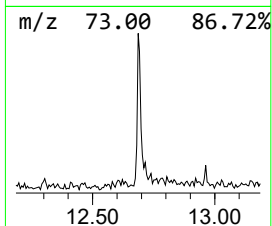
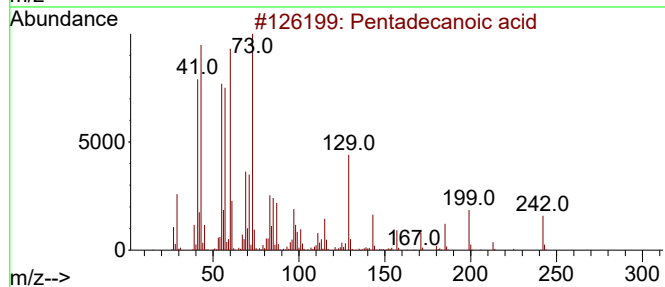
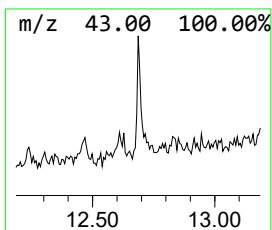
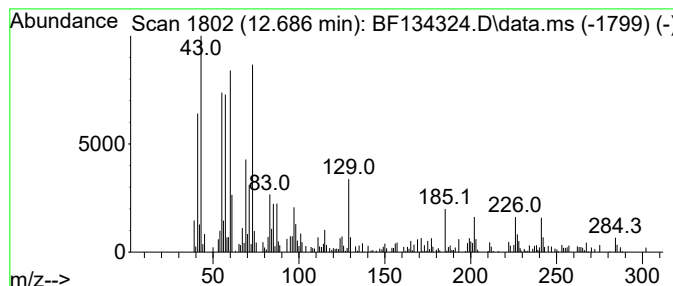
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	5.06 ng	114470	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	96
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Heptadecanoic acid	270	C17H34O2	000506-12-7	89
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134324.D
Acq On : 17 Jul 2023 19:48
Operator : CG\JU
Sample : 03601-01RE
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-1-071223RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.069	2.8	ng	54849	1	6.840	395606	20.0
Ethanol, 2-(2-e...	6.669	3.6	ng	71033	1	6.840	395606	20.0
Pentadecane, 2,...	10.786	2.0	ng	46402	4	11.369	452813	20.0
n-Hexadecanoic ...	11.898	13.4	ng	304146	4	11.369	452813	20.0
Pentadecanoic acid	12.686	5.1	ng	114470	4	11.369	452813	20.0