

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
 Data File : BF126669.D
 Acq On : 25 Jan 2022 17:50
 Operator : CG/JU
 Sample : N1250-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-2

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-BF011822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126669.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	28	34	41	rVB	751338	951198	24.22%	4.258%
2	5.575	589	593	596	rBV	1998282	1722276	43.86%	7.709%
3	6.569	757	762	767	rBV	1341848	1141070	29.06%	5.108%
4	6.963	825	829	832	rVB	855268	719413	18.32%	3.220%
5	7.522	919	924	927	rBV	2289378	2477224	63.08%	11.089%
6	8.245	1043	1047	1050	rBV	1116594	947644	24.13%	4.242%
7	9.322	1224	1230	1233	rBV	4331754	3927194	100.00%	17.579%
8	9.428	1244	1248	1251	rVB2	84559	91755	2.34%	0.411%
9	9.810	1308	1313	1317	rBV4	30083	41665	1.06%	0.187%
10	10.004	1342	1346	1355	rVB	1284205	1059180	26.97%	4.741%
11	10.792	1476	1480	1484	rBV	2503010	2330942	59.35%	10.434%
12	11.492	1596	1599	1603	rBV	1117652	1032029	26.28%	4.620%
13	11.716	1632	1637	1642	rBV2	75404	92505	2.36%	0.414%
14	11.880	1661	1665	1668	rBV	331857	256089	6.52%	1.146%
15	12.010	1683	1687	1692	rBV	40906	46220	1.18%	0.207%
16	12.539	1772	1777	1780	rBV4	38765	47081	1.20%	0.211%
17	12.586	1782	1785	1794	rVB	522094	489719	12.47%	2.192%
18	12.675	1797	1800	1803	rBV	105944	79039	2.01%	0.354%
19	12.733	1805	1810	1813	rBV2	57381	57218	1.46%	0.256%
20	13.086	1865	1870	1873	rBV	3666342	3264804	83.13%	14.614%
21	13.974	2018	2021	2027	rBV2	83708	93164	2.37%	0.417%
22	14.139	2046	2049	2053	rBV	689956	616796	15.71%	2.761%
23	14.463	2101	2104	2107	rBV	74117	67932	1.73%	0.304%
24	15.010	2193	2197	2202	rVB	178526	180355	4.59%	0.807%
25	15.668	2303	2309	2318	rBV	470477	607832	15.48%	2.721%

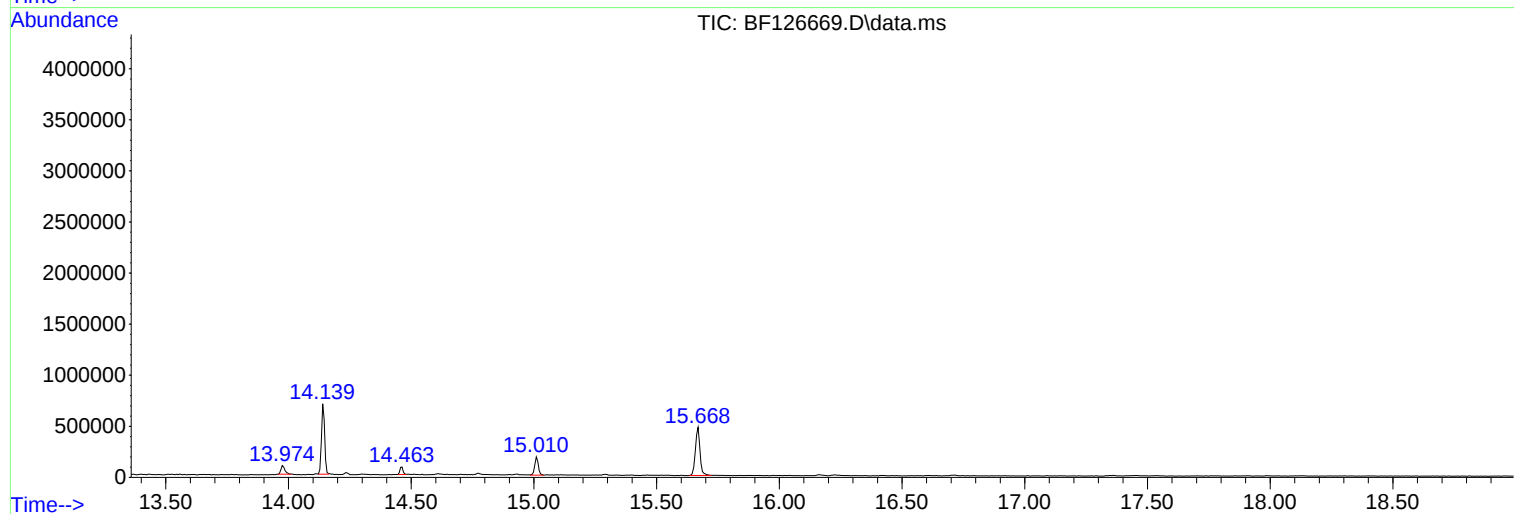
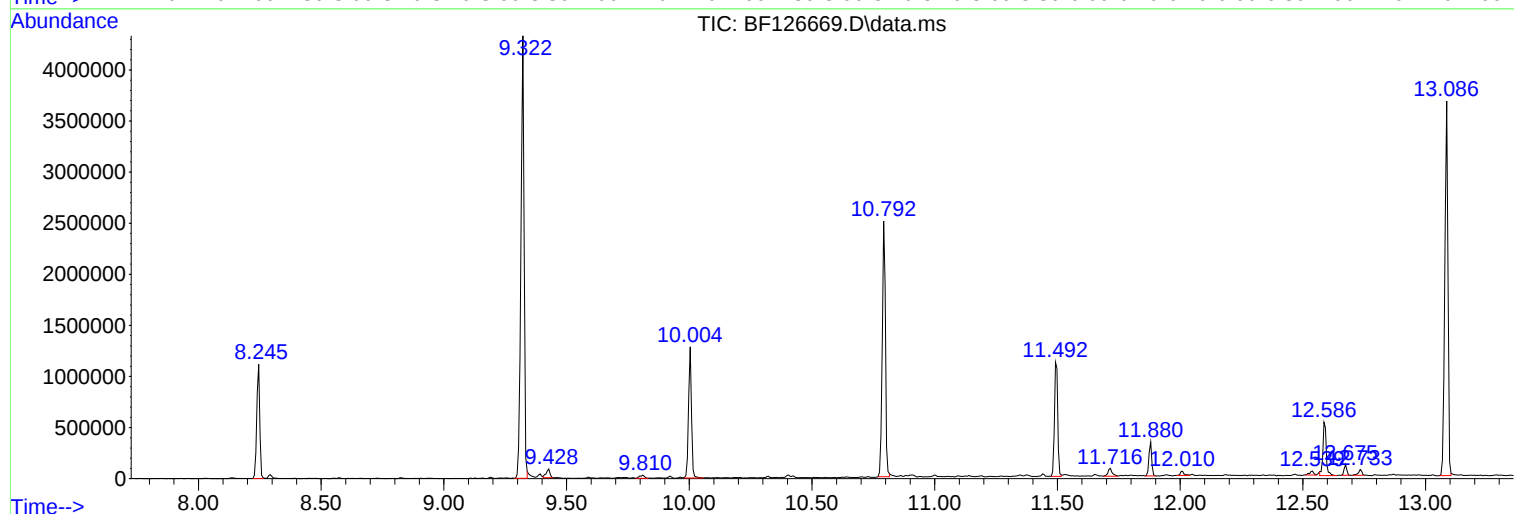
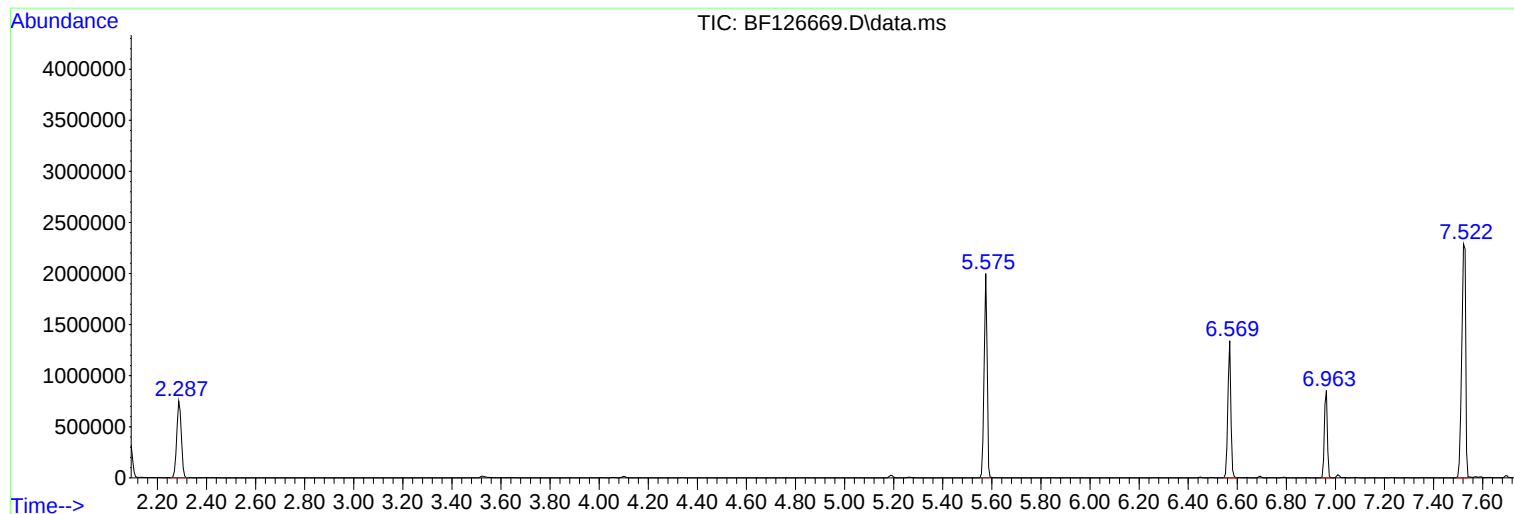
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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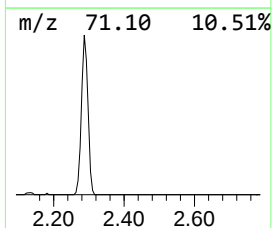
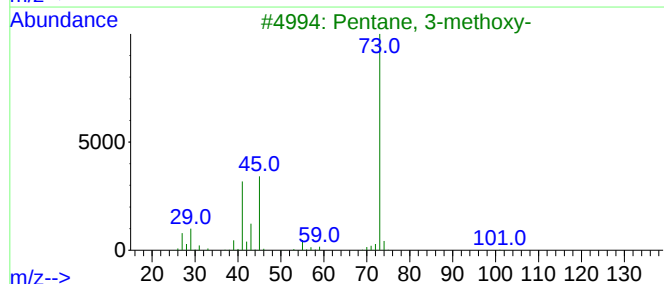
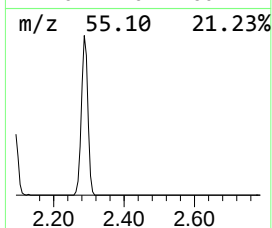
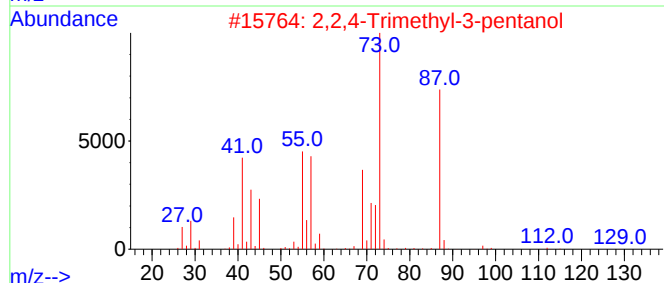
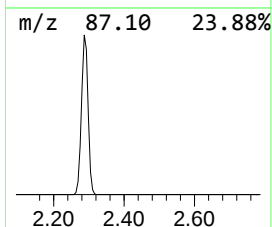
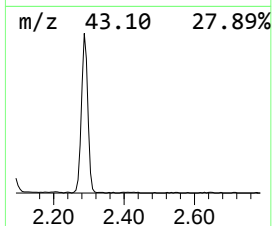
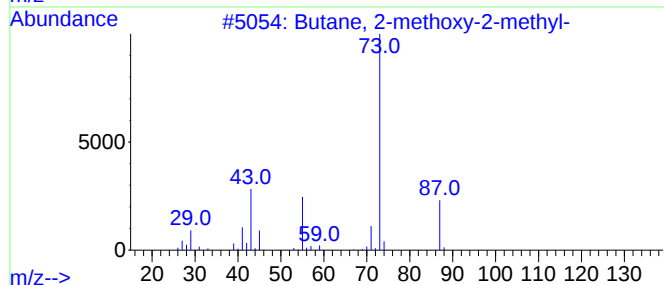
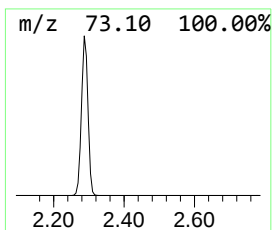
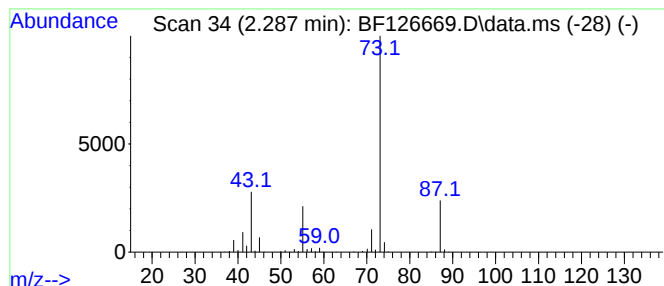
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	26.44 ng	951198	1,4-Dichlorobenzene-d4	6.963

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	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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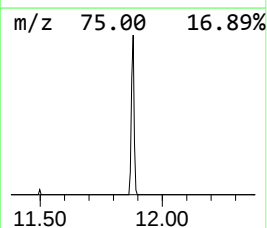
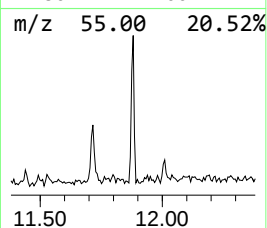
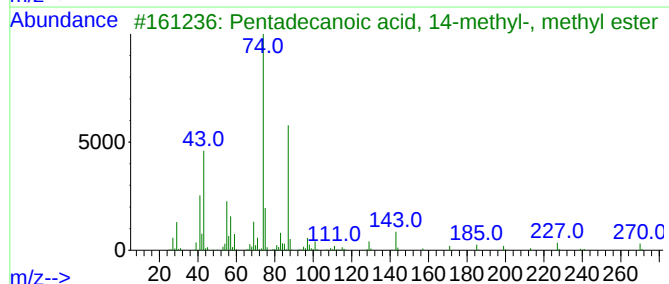
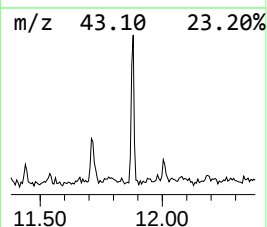
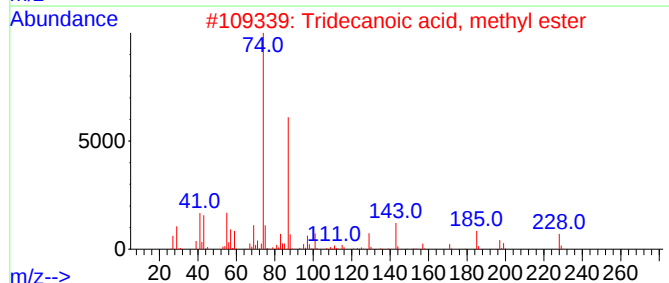
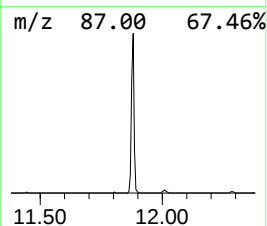
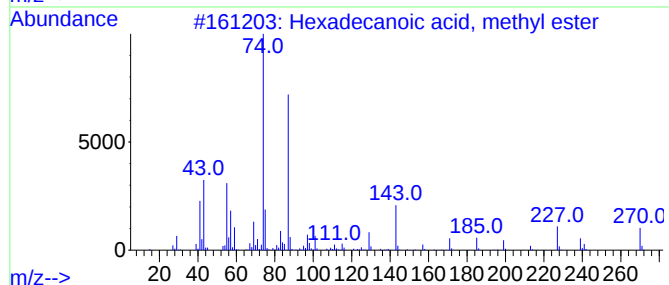
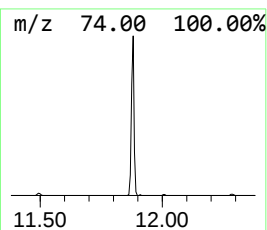
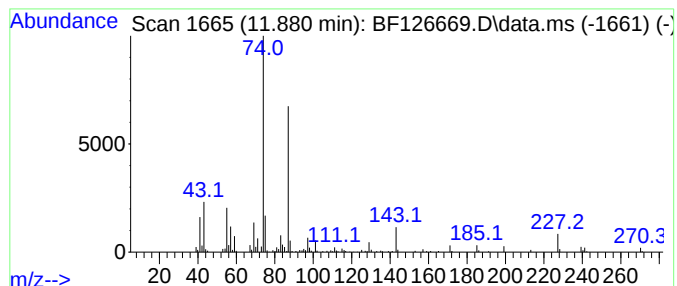
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.881	4.96 ng	256089	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90



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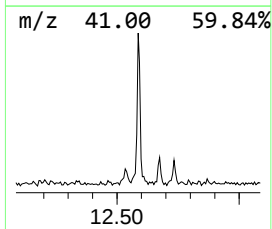
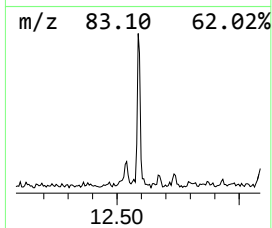
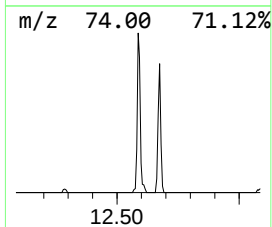
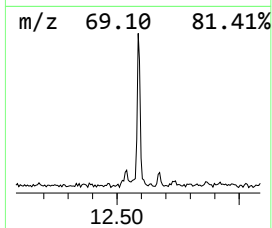
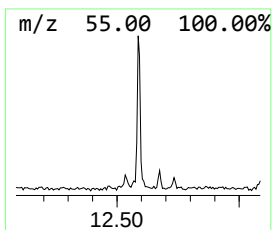
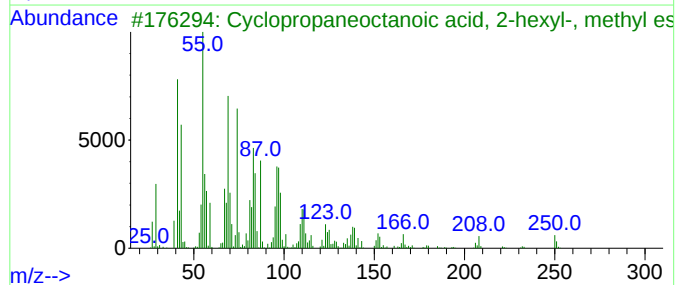
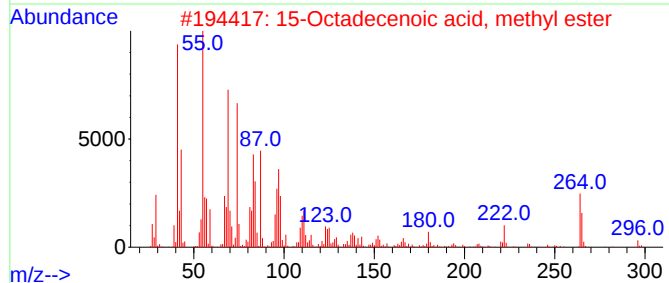
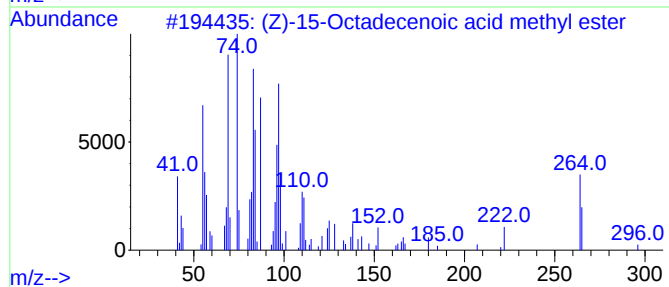
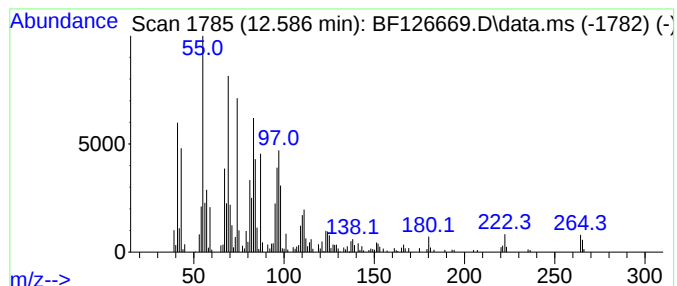
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Peak Number 3 (Z)-15-Octadecenoic acid me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	9.49 ng	489719	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	68
2			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	68
3			Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	64
4			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	64
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	62



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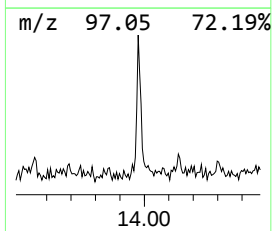
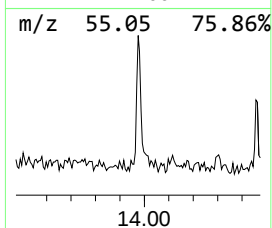
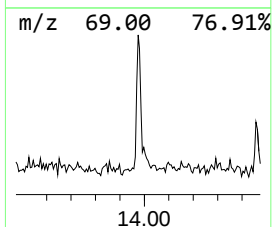
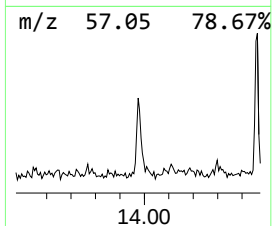
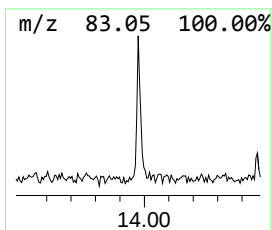
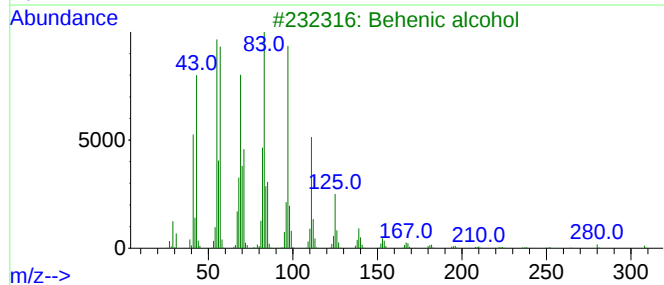
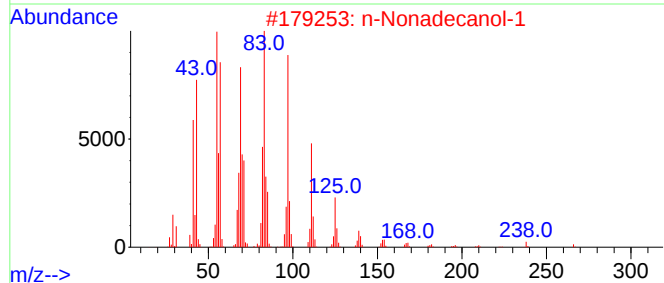
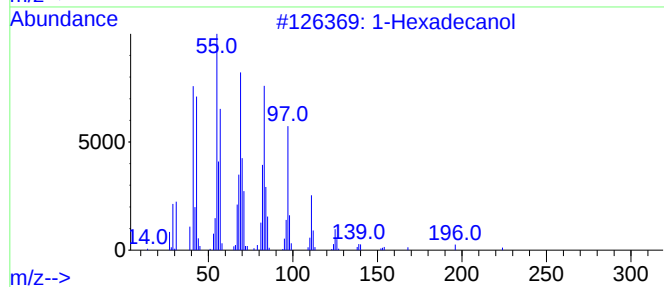
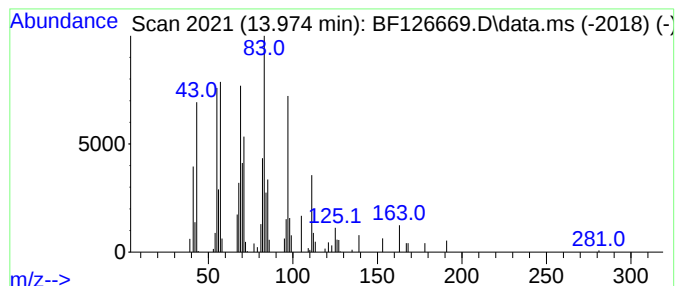
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Peak Number 4 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	3.02 ng	93164	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	87
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Behenic alcohol	326	C22H46O	000661-19-8	83
4			1-Hexacosene	364	C26H52	018835-33-1	81
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81



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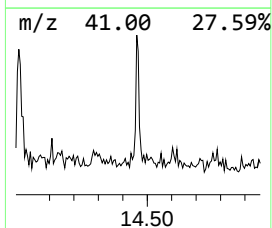
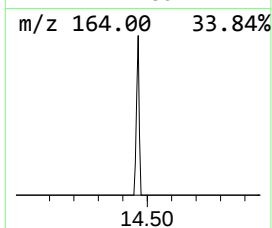
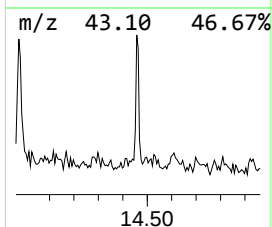
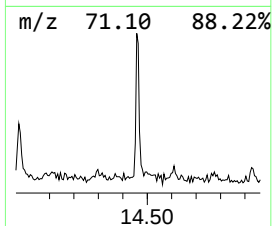
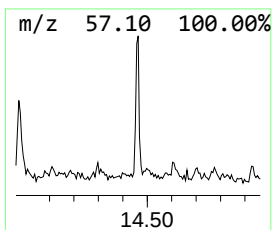
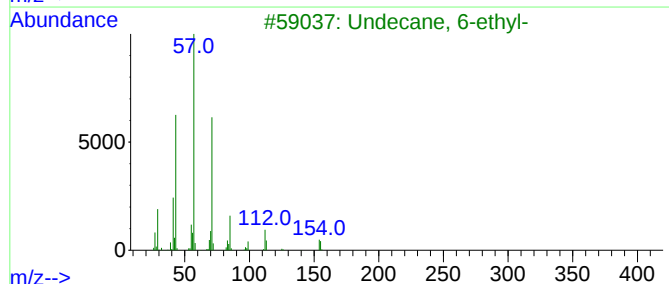
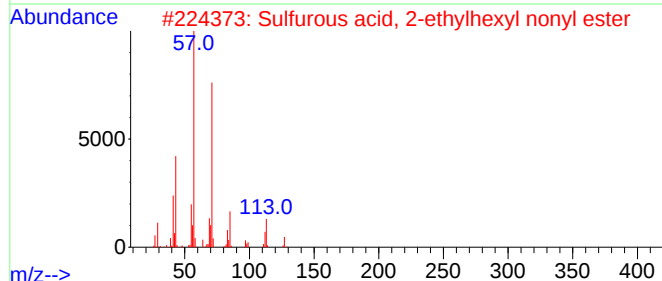
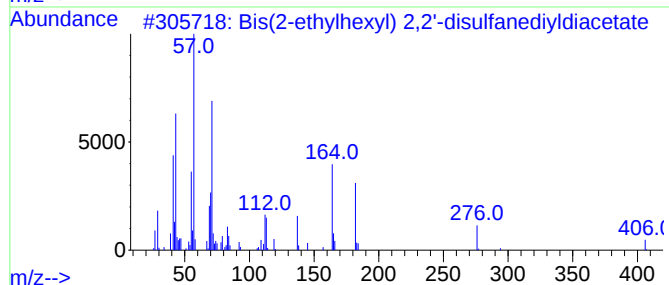
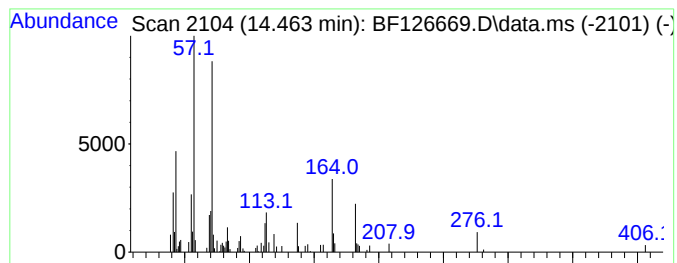
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Peak Number 5 Bis(2-ethylhexyl) 2,2'-disu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.20 ng	67932	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) 2,2'-disulfane...	406	C20H38O4S2	062268-47-7	99
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	46
3			Undecane, 6-ethyl-	184	C13H28	017312-60-6	43
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	43
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	43



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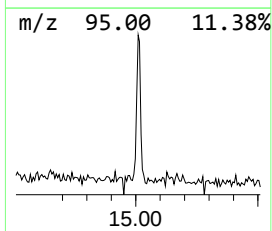
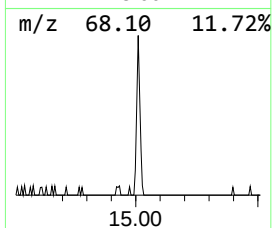
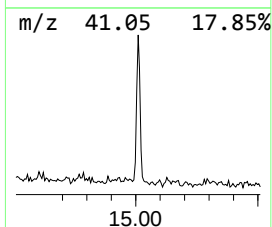
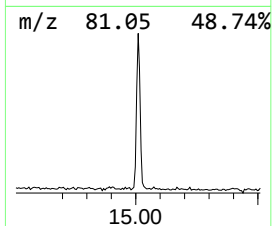
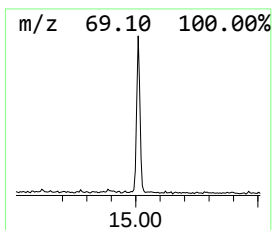
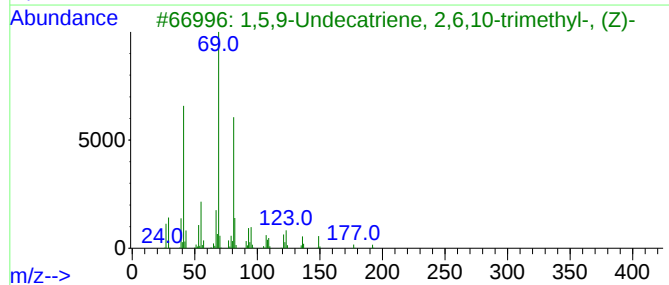
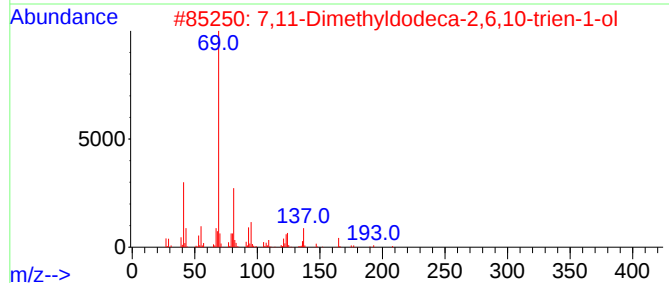
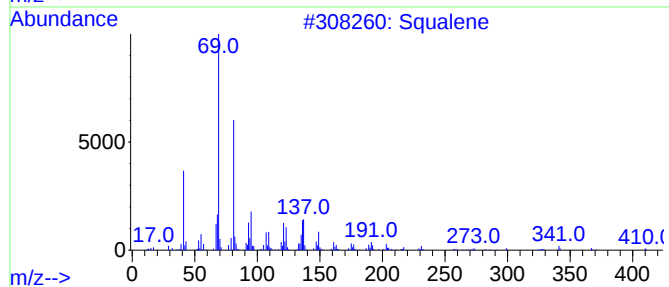
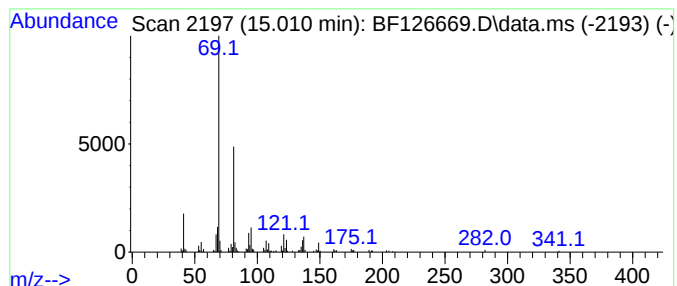
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.010	5.93 ng	180355	Perylene-d12	15.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	83
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78
4			(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	72
5			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
Data File : BF126669.D
Acq On : 25 Jan 2022 17:50
Operator : CG/JU
Sample : N1250-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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
Butane, 2-metho...	2.287	26.4	ng	951198	1	6.963	719413	20.0
Hexadecanoic ac...	11.881	5.0	ng	256089	4	11.492	1032030	20.0
(Z)-15-Octadece...	12.586	9.5	ng	489719	4	11.492	1032030	20.0
1-Hexadecanol	13.974	3.0	ng	93164	5	14.139	616796	20.0
Bis(2-ethylhexy...	14.463	2.2	ng	67932	5	14.139	616796	20.0
Squalene	15.010	5.9	ng	180355	6	15.668	607832	20.0