

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
 Data File : BF140998.D
 Acq On : 27 Dec 2024 16:03
 Operator : RC/JU
 Sample : P5299-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02

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-BF122624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.893	297	306	315	rBV	56114	95906	1.31%	0.175%
2	5.046	492	502	508	rVB	47169	83271	1.13%	0.152%
3	5.434	561	568	573	rBV	4512168	6146107	83.65%	11.222%
4	6.440	732	739	745	rBV	4467023	6331156	86.17%	11.560%
5	6.822	799	804	810	rVB	1232077	1512528	20.59%	2.762%
6	7.381	890	899	904	rBV	3001706	4021656	54.73%	7.343%
7	7.422	904	906	910	rVB	70753	77659	1.06%	0.142%
8	7.639	938	943	950	rVB2	138497	195688	2.66%	0.357%
9	8.104	1012	1022	1027	rBV	1611546	2281149	31.05%	4.165%
10	8.169	1027	1033	1036	rVB	86185	115295	1.57%	0.211%
11	8.316	1054	1058	1066	rVB4	58046	109580	1.49%	0.200%
12	8.398	1066	1072	1078	rBV4	74582	158812	2.16%	0.290%
13	8.481	1083	1086	1090	rVV2	59223	83887	1.14%	0.153%
14	8.528	1090	1094	1103	rVB	150059	237971	3.24%	0.434%
15	8.698	1118	1123	1127	rVV	342487	450543	6.13%	0.823%
16	8.792	1136	1139	1143	rVB2	65722	83813	1.14%	0.153%
17	8.986	1167	1172	1173	rBV2	70143	98345	1.34%	0.180%
18	9.063	1181	1185	1188	rBV	67494	77930	1.06%	0.142%
19	9.128	1193	1196	1199	rVV	192227	224866	3.06%	0.411%
20	9.181	1199	1205	1209	rVB	5047657	7026377	95.63%	12.829%
21	9.263	1214	1219	1224	rBV	548122	719770	9.80%	1.314%
22	9.581	1268	1273	1281	rVB2	158452	289845	3.94%	0.529%
23	9.792	1305	1309	1313	rVB	199483	245284	3.34%	0.448%
24	9.857	1313	1320	1325	rVB	1759246	2313587	31.49%	4.224%
25	10.569	1435	1441	1447	rBV	860677	1087363	14.80%	1.985%
26	10.639	1447	1453	1467	rBV	3406005	4560799	62.07%	8.327%
27	11.339	1567	1572	1579	rVV	1903833	2349662	31.98%	4.290%
28	11.410	1579	1584	1588	rVB2	91688	117421	1.60%	0.214%
29	11.874	1654	1663	1677	rBV2	801438	1315974	17.91%	2.403%
30	12.574	1774	1782	1790	rBV5	41354	126072	1.72%	0.230%
31	12.657	1791	1796	1808	rVV	201357	332185	4.52%	0.607%
32	12.927	1836	1842	1848	rBV	5453407	7347570	100.00%	13.416%
33	13.510	1937	1941	1948	rVB	50790	79378	1.08%	0.145%
34	13.833	1991	1996	2013	rBV	558557	907712	12.35%	1.657%
35	13.980	2015	2021	2029	rBV	1313759	1754927	23.88%	3.204%
36	14.163	2048	2052	2061	rVB	62364	84977	1.16%	0.155%

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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-BF122624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.474	2101	2105	2119	rBV2	66412	127556	1.74%	0.233%
38	14.857	2167	2170	2177	rVB	57131	80869	1.10%	0.148%
39	15.445	2264	2270	2277	rBV	924074	1435631	19.54%	2.621%
40	15.992	2359	2363	2372	rVB4	42500	80034	1.09%	0.146%

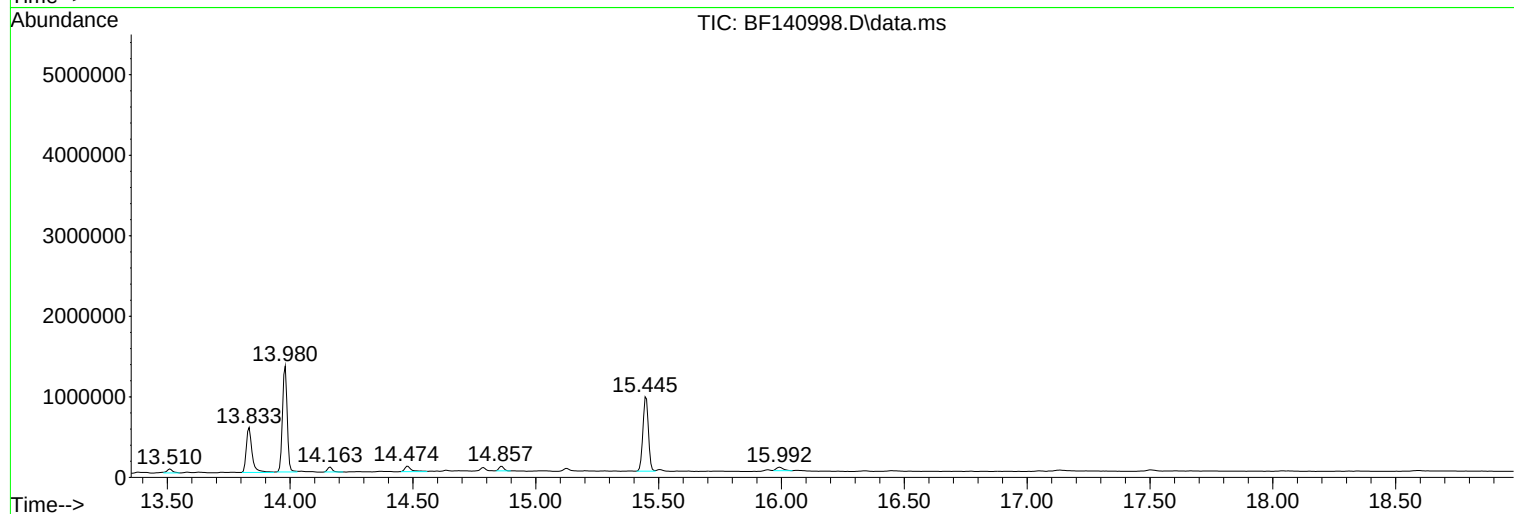
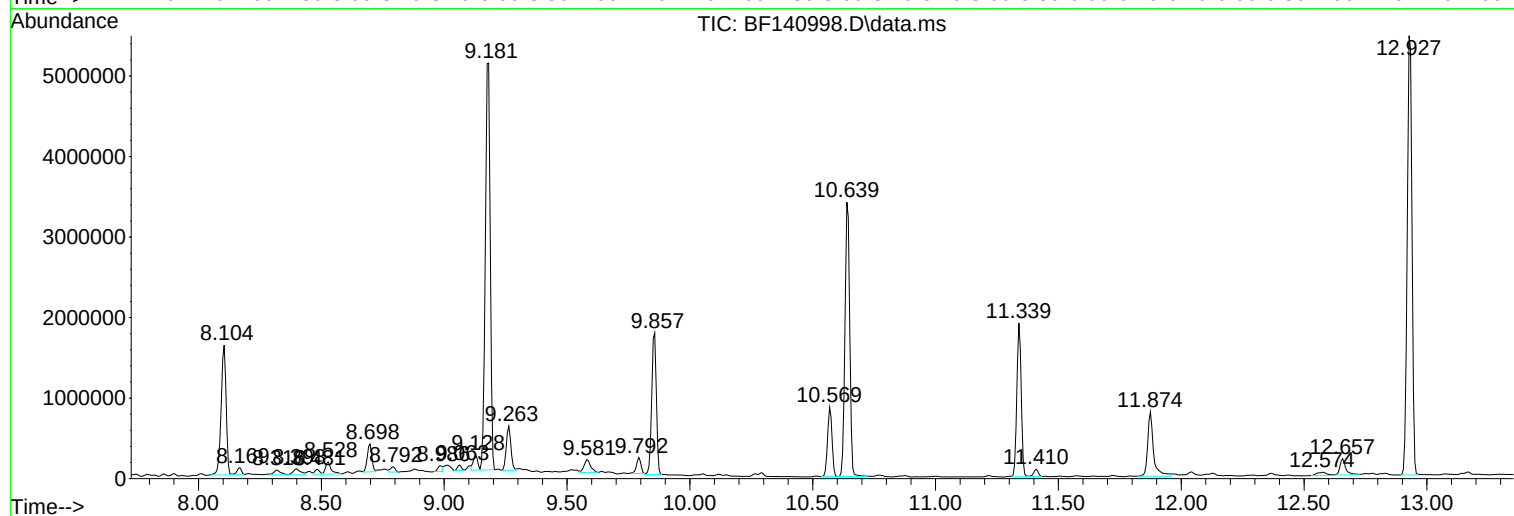
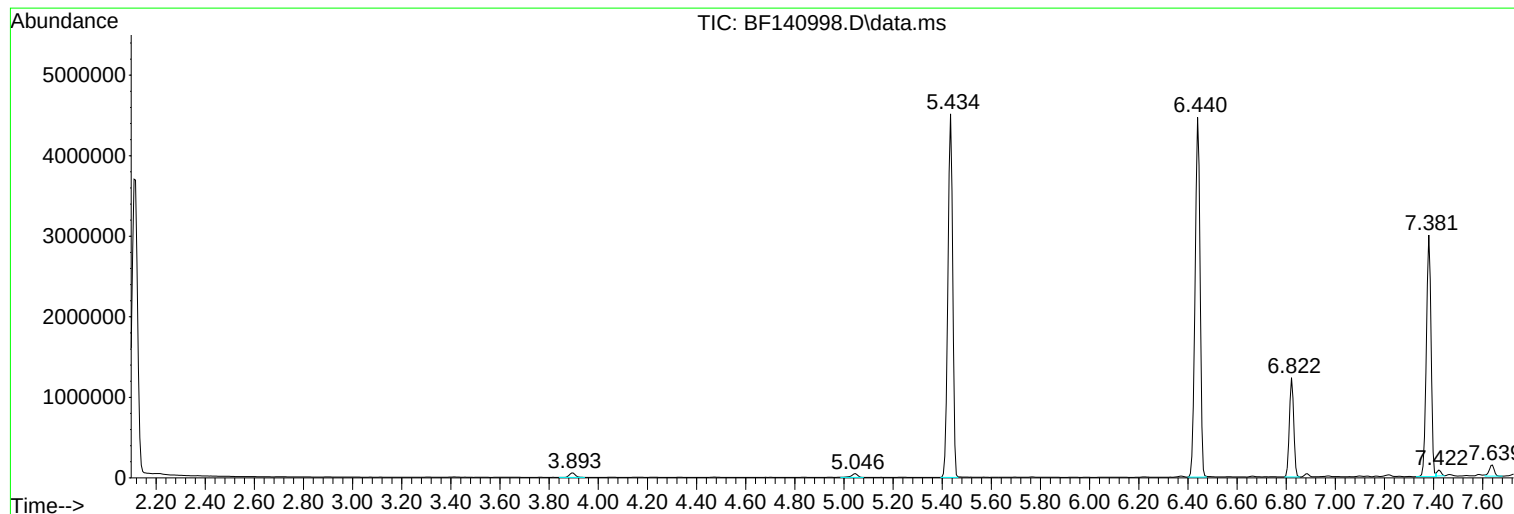
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
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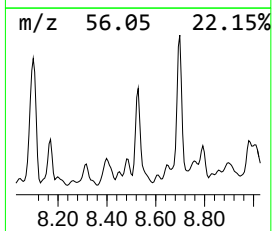
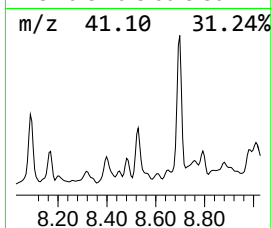
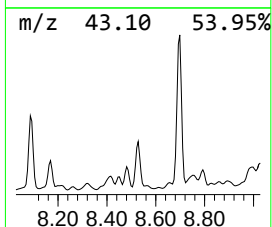
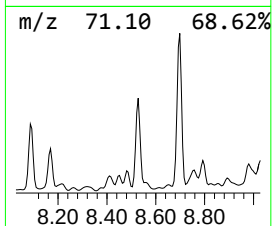
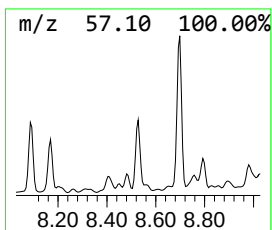
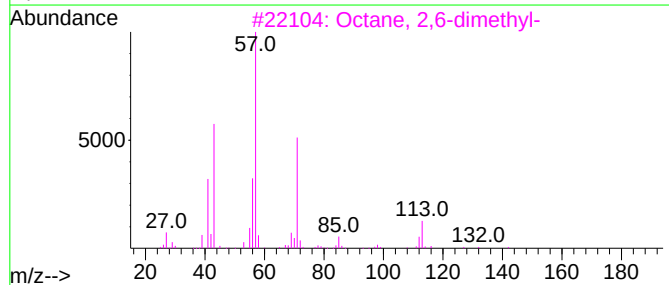
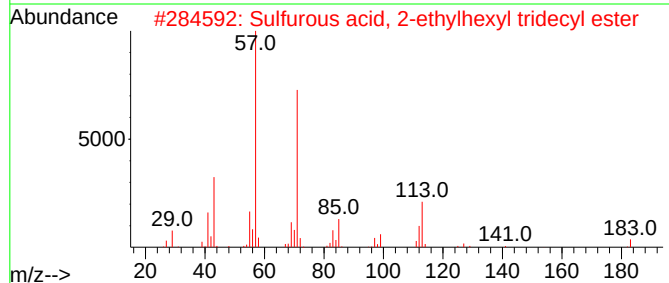
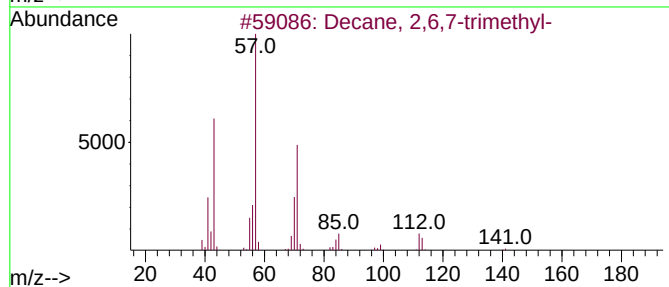
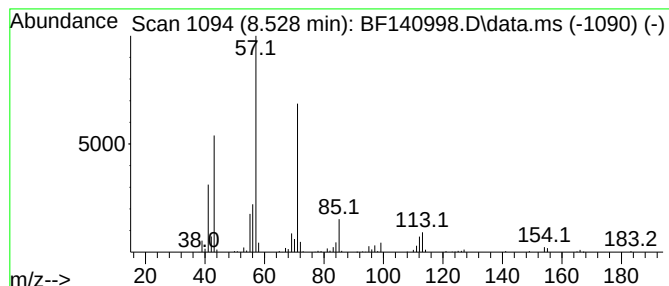
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Decane, 2,6,7-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.528	2.09 ng	237971	Naphthalene-d8	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	78
2		Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	72
3		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64



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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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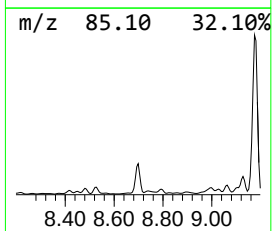
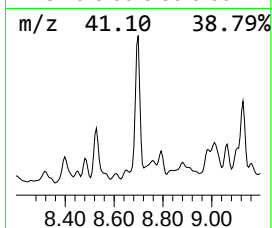
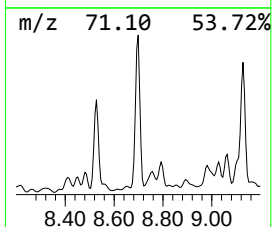
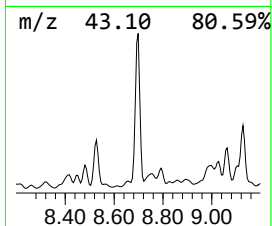
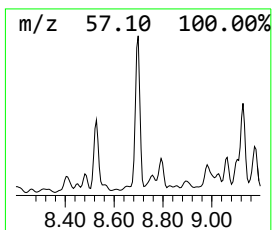
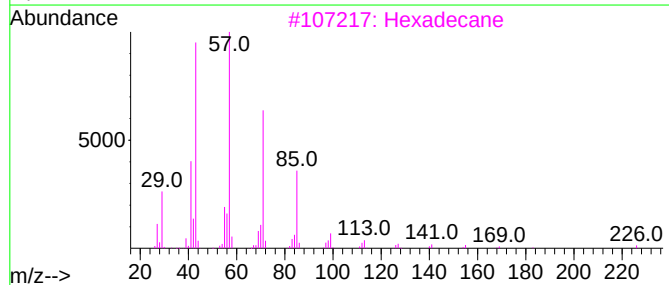
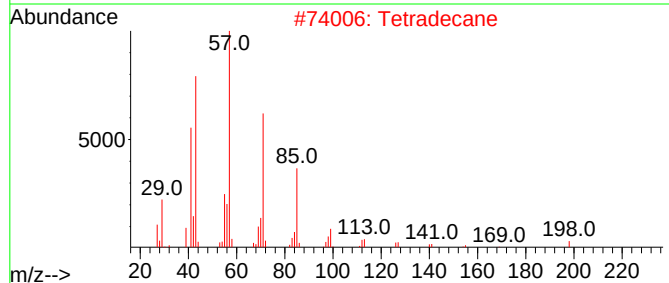
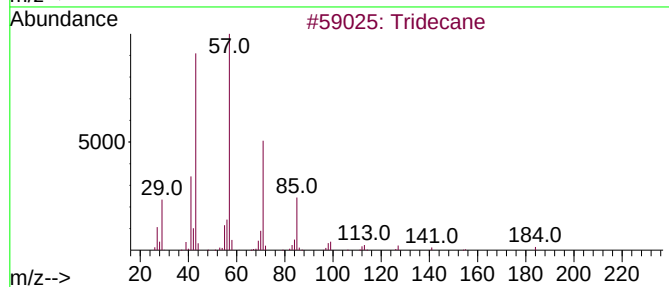
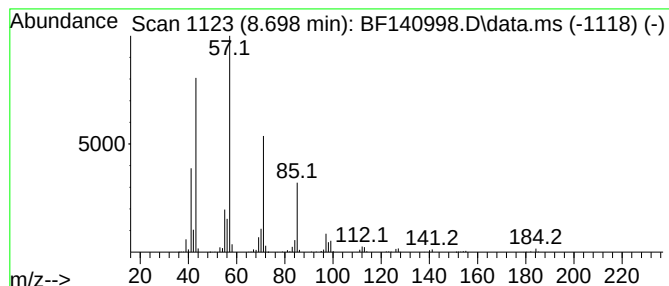
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.698	3.95 ng	450543	Naphthalene-d8	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	93
2		Tetradecane	198	C14H30	000629-59-4	86
3		Hexadecane	226	C16H34	000544-76-3	80
4		Dodecane	170	C12H26	000112-40-3	78
5		Pentadecane	212	C15H32	000629-62-9	78



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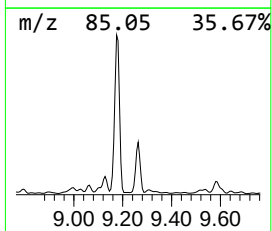
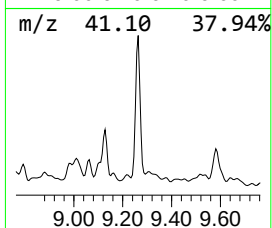
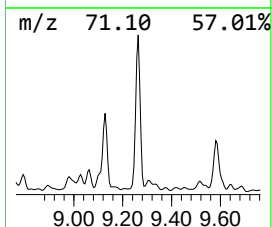
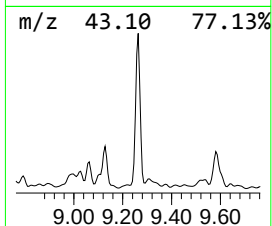
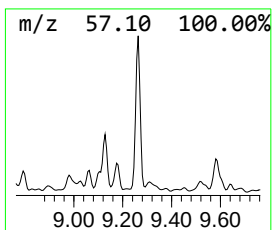
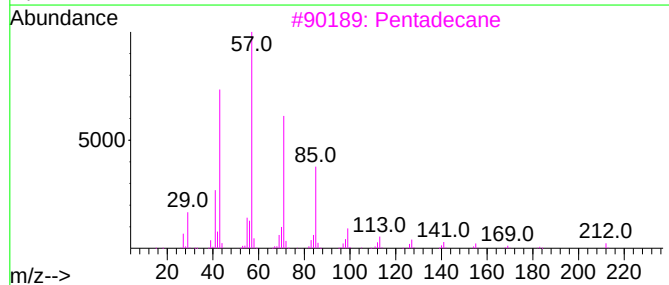
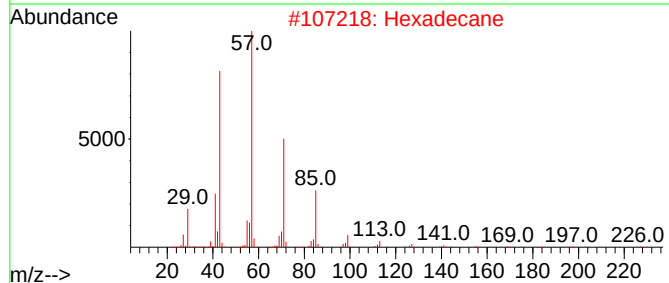
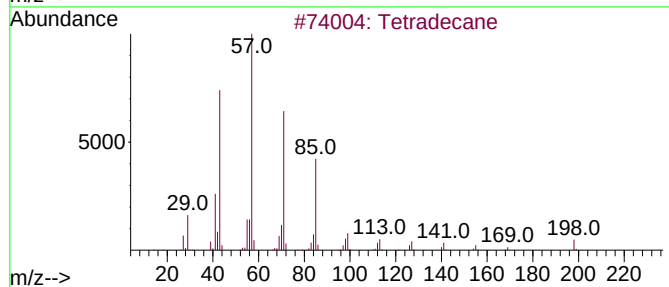
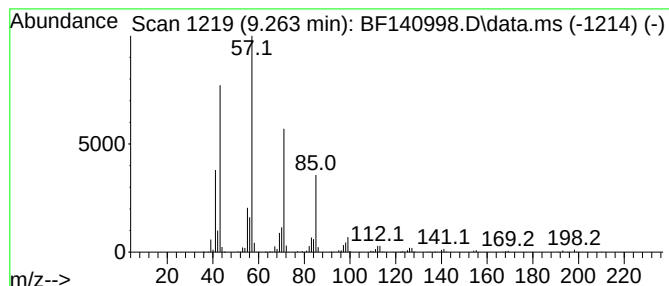
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	6.22 ng	719770	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	96
2			Hexadecane	226	C16H34	000544-76-3	91
3			Pentadecane	212	C15H32	000629-62-9	90
4			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	80
5			Tridecane, 6-methyl-	198	C14H30	013287-21-3	74



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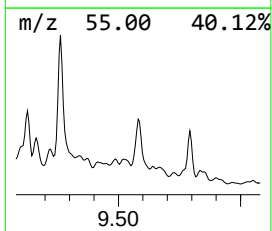
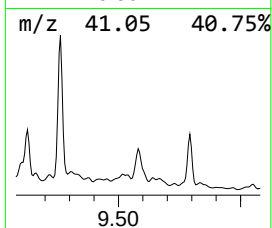
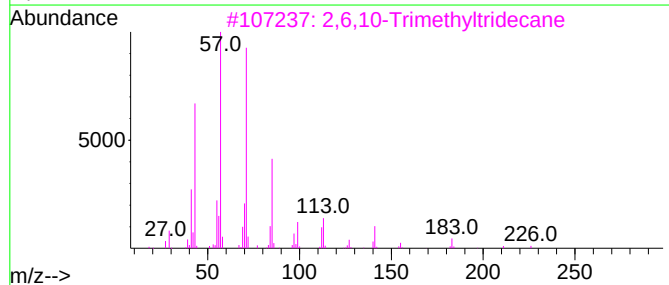
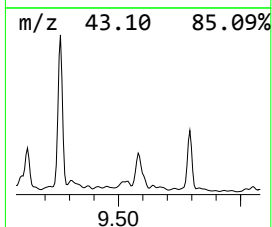
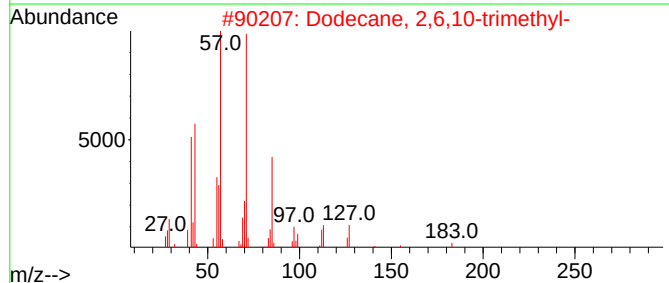
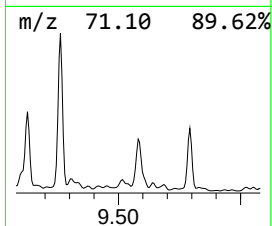
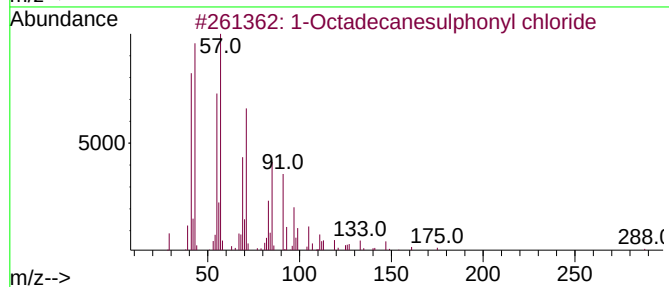
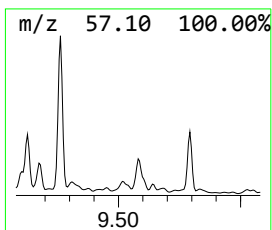
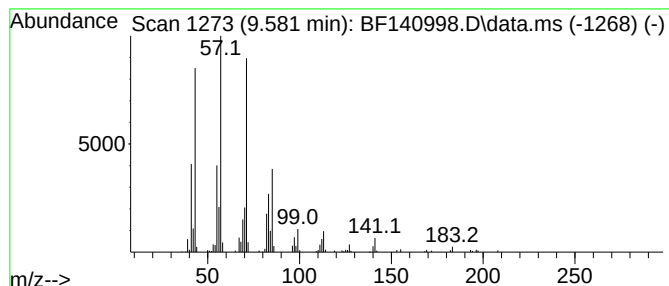
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Octadecanesulphonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.581	2.51 ng	289845	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
3			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	80
4			Hexadecane	226	C16H34	000544-76-3	80
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74



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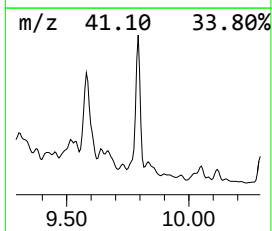
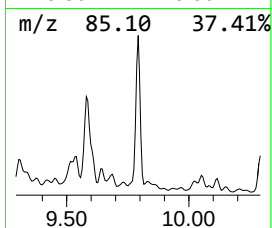
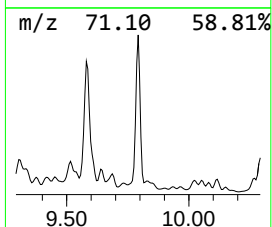
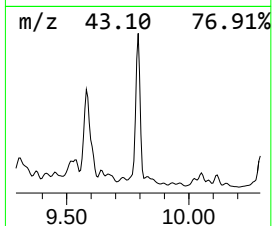
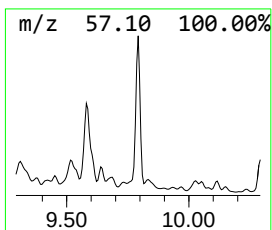
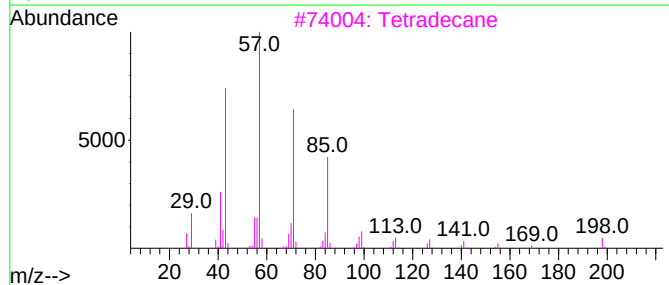
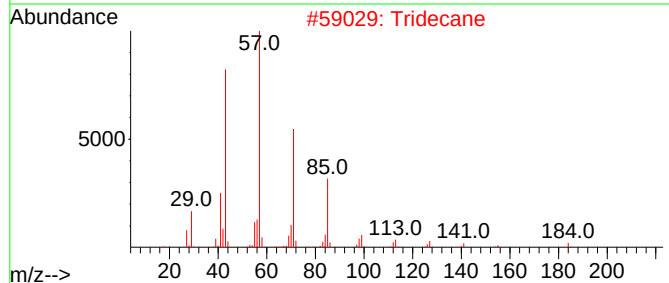
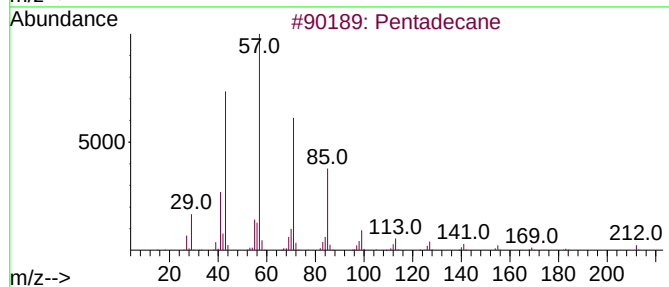
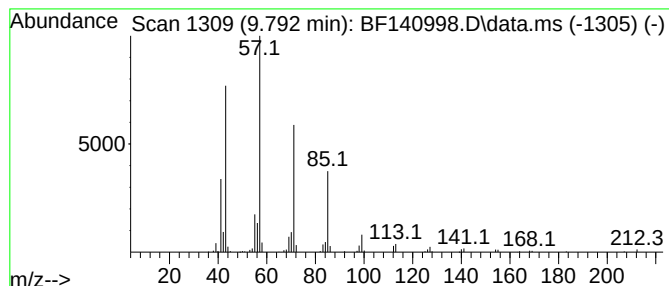
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	2.12 ng	245284	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	95
2			Tridecane	184	C13H28	000629-50-5	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF140998.D
Acq On : 27 Dec 2024 16:03
Operator : RC/JU
Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

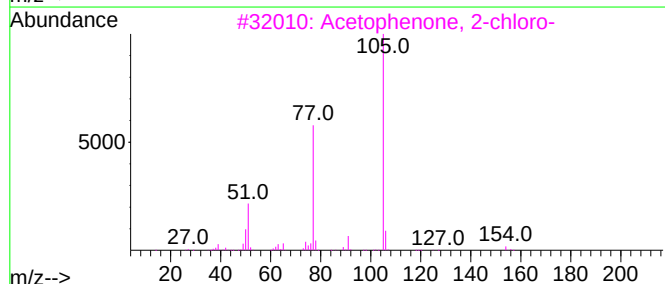
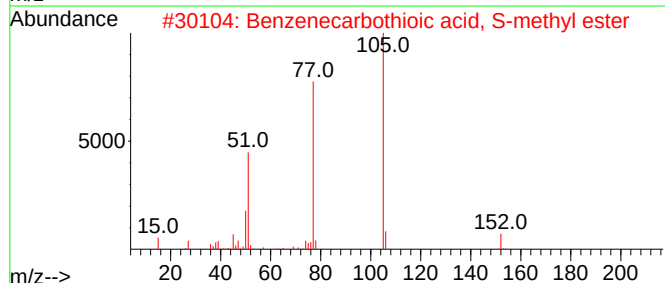
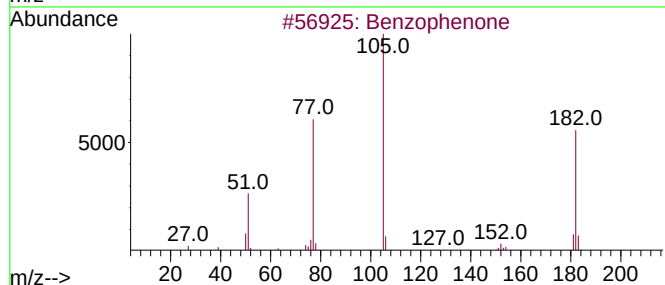
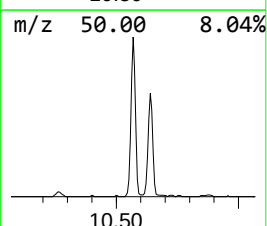
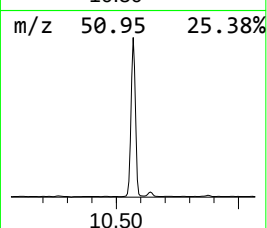
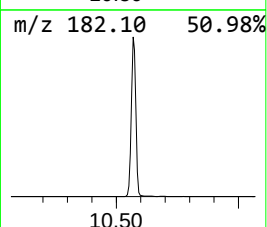
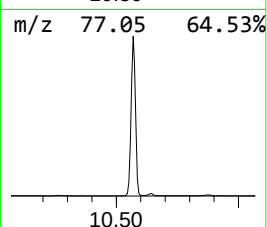
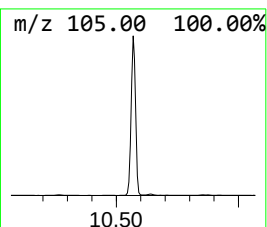
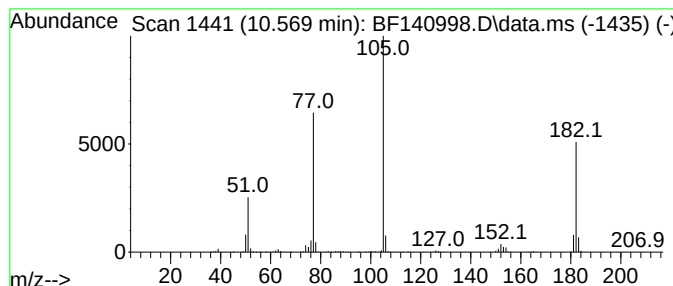
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	9.40 ng	1087360	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF140998.D
Acq On : 27 Dec 2024 16:03
Operator : RC/JU
Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

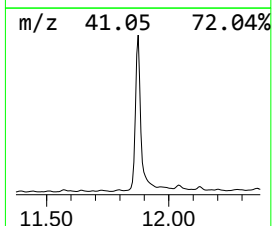
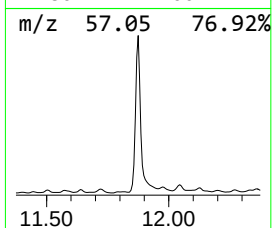
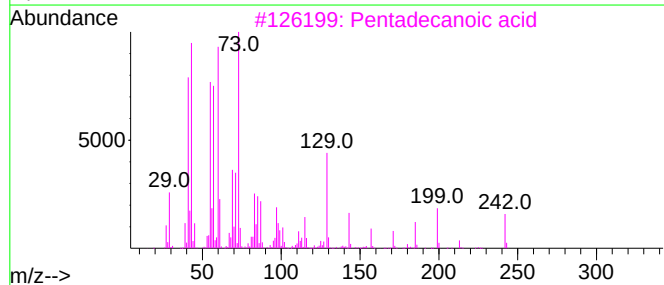
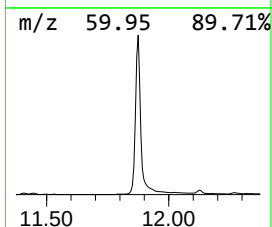
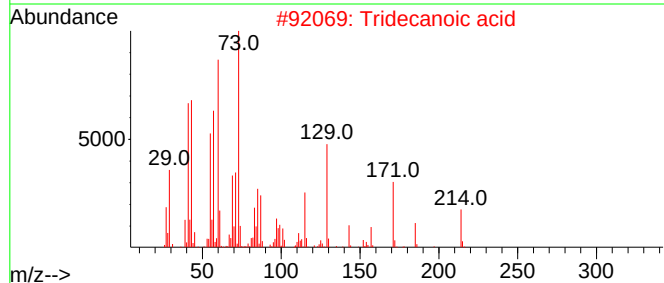
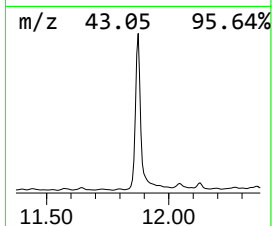
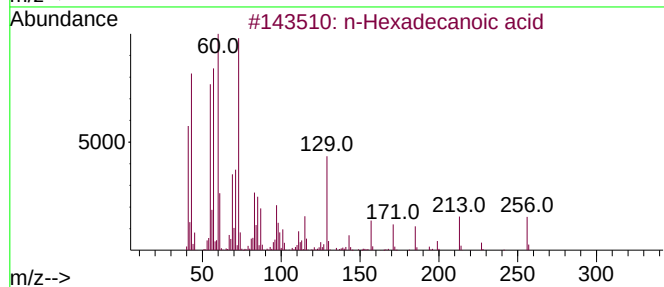
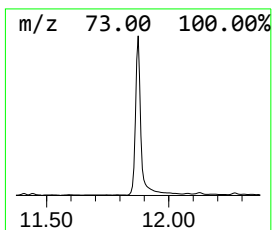
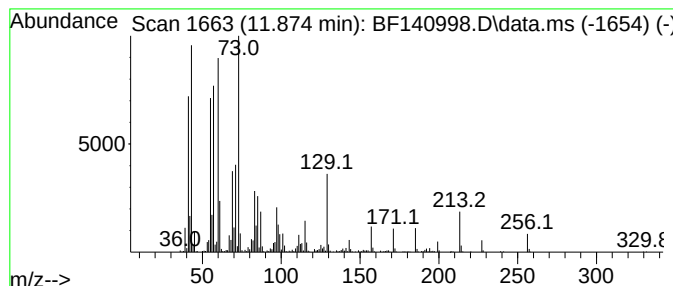
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	11.20 ng	1315970	Phenanthrene-d10	11.339

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF140998.D
Acq On : 27 Dec 2024 16:03
Operator : RC/JU
Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

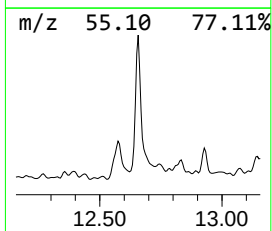
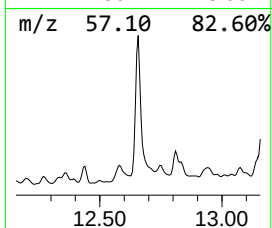
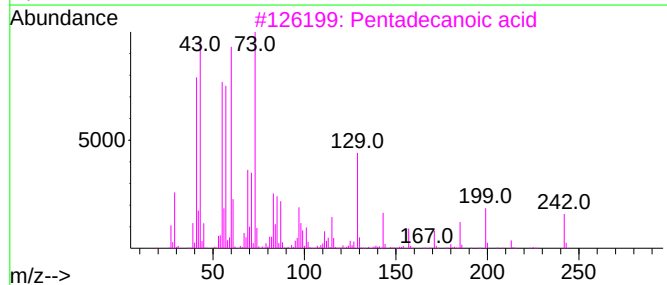
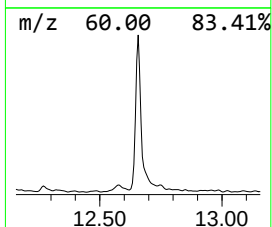
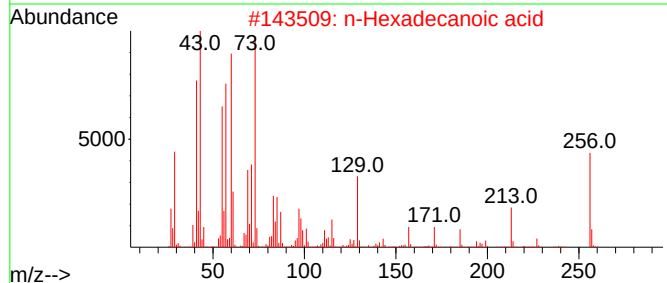
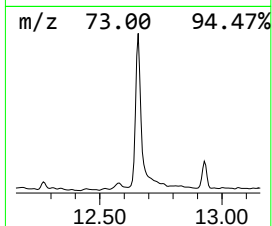
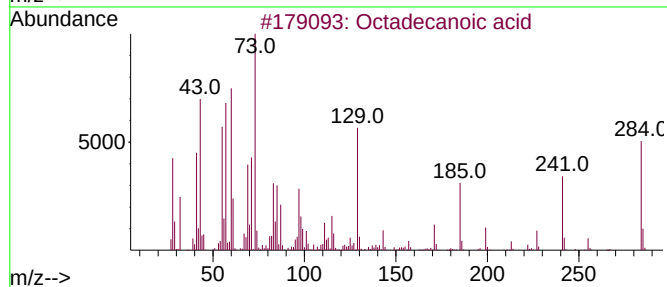
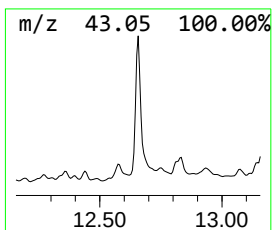
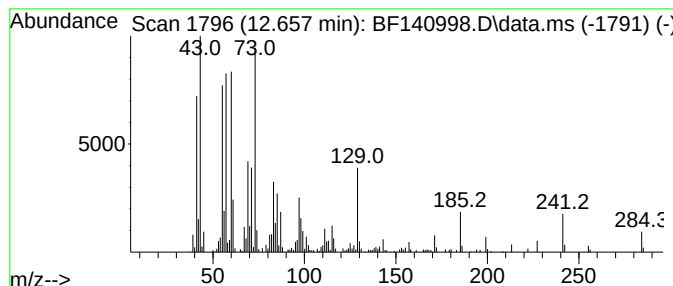
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.83 ng	332185	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF140998.D
Acq On : 27 Dec 2024 16:03
Operator : RC/JU
Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

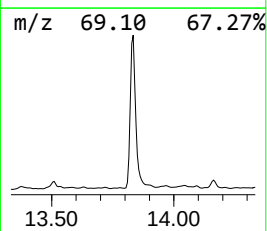
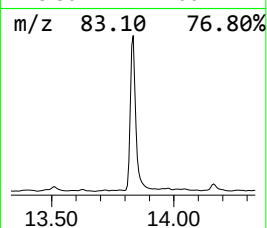
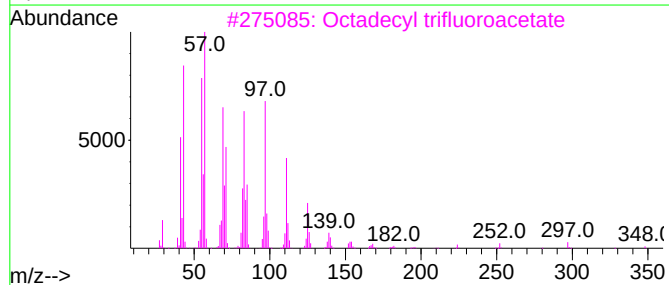
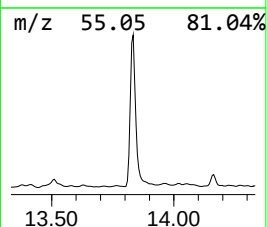
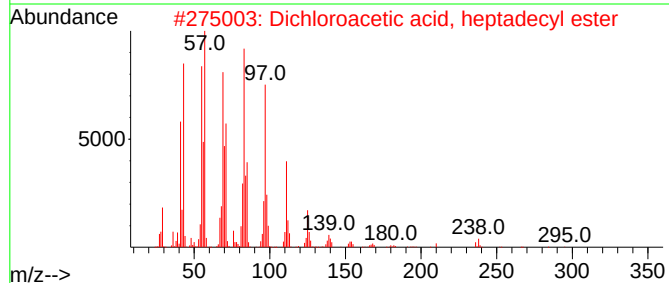
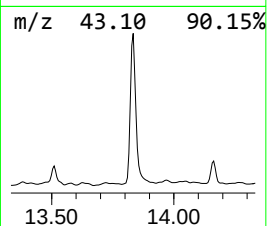
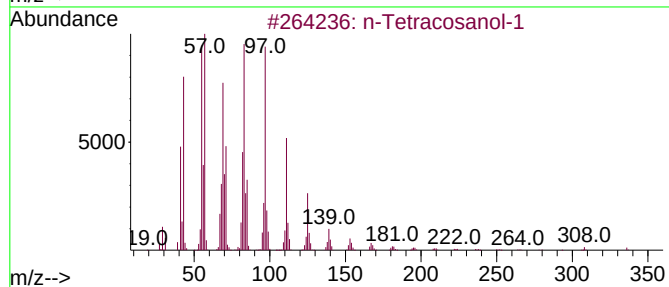
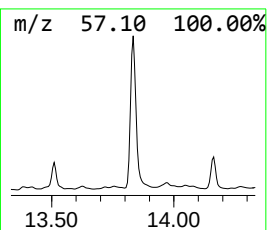
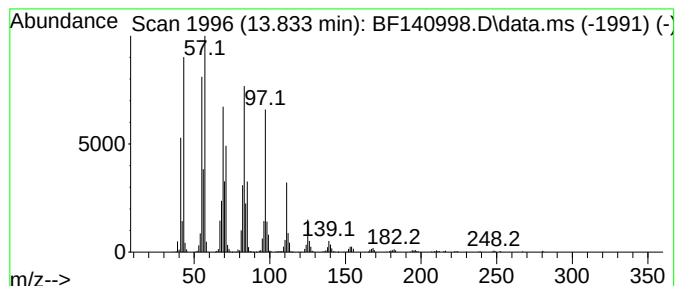
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	10.34 ng	907712	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4			Octacosanol	410	C28H58O	000557-61-9	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122724\
Data File : BF140998.D
Acq On : 27 Dec 2024 16:03
Operator : RC/JU
Sample : P5299-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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
Decane, 2,6,7-t...	8.528	2.1	ng	237971	2	8.104	2281150	20.0
Tridecane	8.698	4.0	ng	450543	2	8.104	2281150	20.0
Tetradecane	9.263	6.2	ng	719770	3	9.857	2313590	20.0
1-Octadecanesul...	9.581	2.5	ng	289845	3	9.857	2313590	20.0
Pentadecane	9.792	2.1	ng	245284	3	9.857	2313590	20.0
Benzophenone	10.569	9.4	ng	1087360	3	9.857	2313590	20.0
n-Hexadecanoic ...	11.874	11.2	ng	1315970	4	11.339	2349660	20.0
Octadecanoic acid	12.657	2.8	ng	332185	4	11.339	2349660	20.0
n-Tetracosanol-1	13.833	10.3	ng	907712	5	13.980	1754930	20.0