

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061721\
 Data File : BF124357.D
 Acq On : 17 Jun 2021 11:38
 Operator : JU/CG
 Sample : M2678-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPLP-AMND-COMP-D(CL-01A)

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	490	492	499	rBB2	18943	20765	1.10%	0.228%
2	5.404	561	564	575	rBV	474429	455622	24.09%	5.001%
3	6.428	735	738	752	rBB	269690	272117	14.39%	2.987%
4	6.781	795	798	803	rBB	300382	227774	12.05%	2.500%
5	7.351	890	895	898	rBV	907341	851604	45.04%	9.348%
6	8.063	1013	1016	1020	rBV	337529	296152	15.66%	3.251%
7	9.145	1196	1200	1203	rBV	2140242	1657394	87.65%	18.193%
8	9.292	1222	1225	1235	rVB	119421	111293	5.89%	1.222%
9	9.822	1311	1315	1318	rBV	505289	366258	19.37%	4.020%
10	10.586	1442	1445	1446	rBV	52196	46760	2.47%	0.513%
11	10.616	1446	1450	1453	rVB	1434714	1143185	60.45%	12.548%
12	11.310	1564	1568	1572	rBV	514754	404328	21.38%	4.438%
13	11.839	1654	1658	1665	rBV2	76608	85975	4.55%	0.944%
14	12.621	1788	1791	1805	rVB6	35527	77123	4.08%	0.847%
15	12.904	1834	1839	1842	rBV	1923956	1890982	100.00%	20.757%
16	13.174	1878	1885	1886	rBV3	23082	38116	2.02%	0.418%
17	13.192	1886	1888	1897	rVB4	31216	60789	3.21%	0.667%
18	13.957	2014	2018	2021	rVB	395410	339970	17.98%	3.732%
19	14.245	2057	2067	2074	rBV4	41051	104489	5.53%	1.147%
20	14.415	2091	2096	2100	rBV2	16740	20562	1.09%	0.226%
21	14.721	2142	2148	2150	rBV3	34998	43402	2.30%	0.476%
22	14.992	2186	2194	2195	rBV6	23099	33449	1.77%	0.367%
23	15.010	2195	2197	2201	rVV4	23369	33949	1.80%	0.373%
24	15.051	2201	2204	2207	rVB2	29061	28830	1.52%	0.316%
25	15.410	2255	2265	2275	rVB	232853	344367	18.21%	3.780%
26	15.851	2335	2340	2348	rVB4	42249	90424	4.78%	0.993%
27	16.345	2416	2424	2428	rBV4	22654	41316	2.18%	0.454%
28	16.921	2518	2522	2527	rVB5	13127	23291	1.23%	0.256%

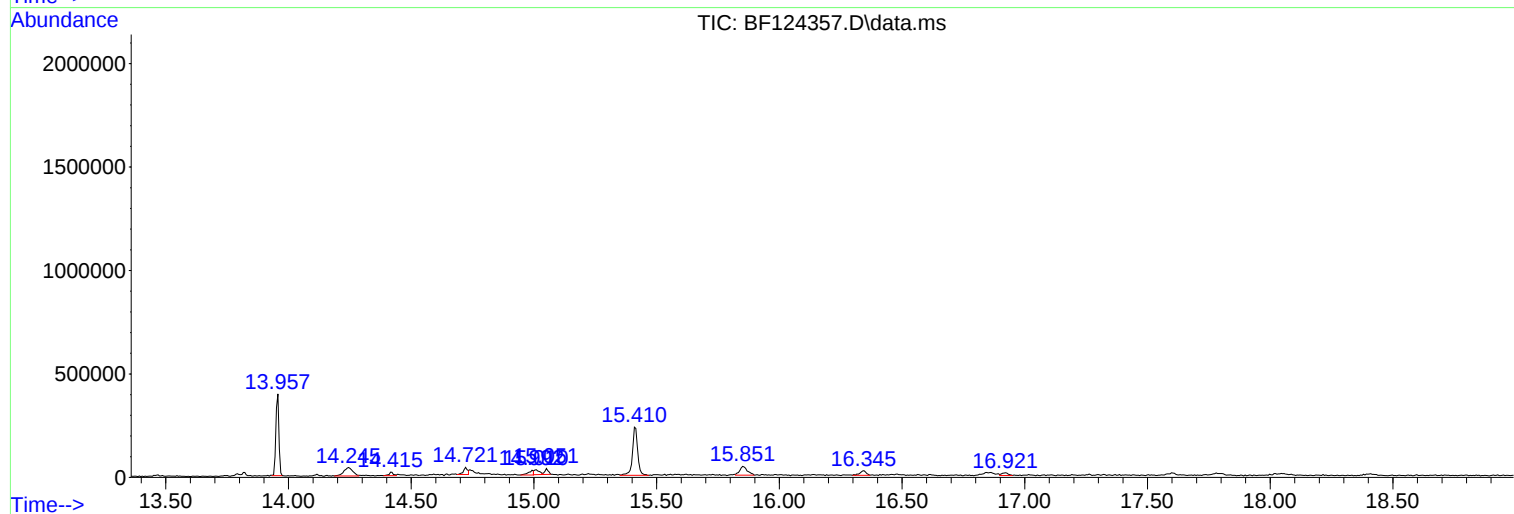
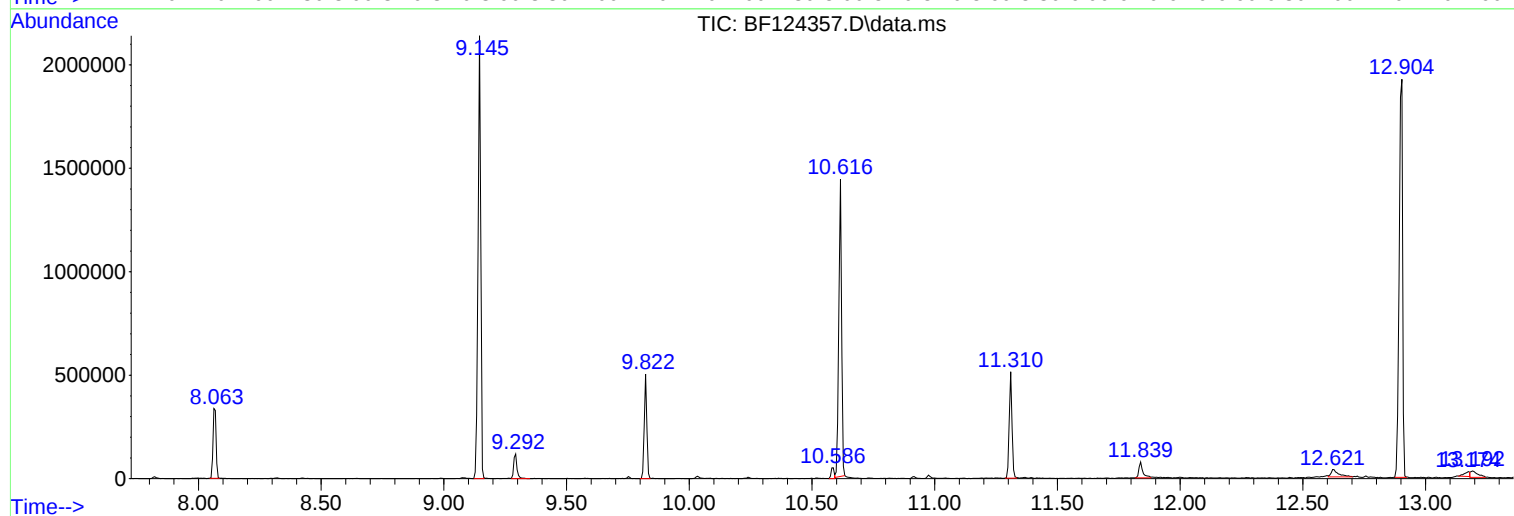
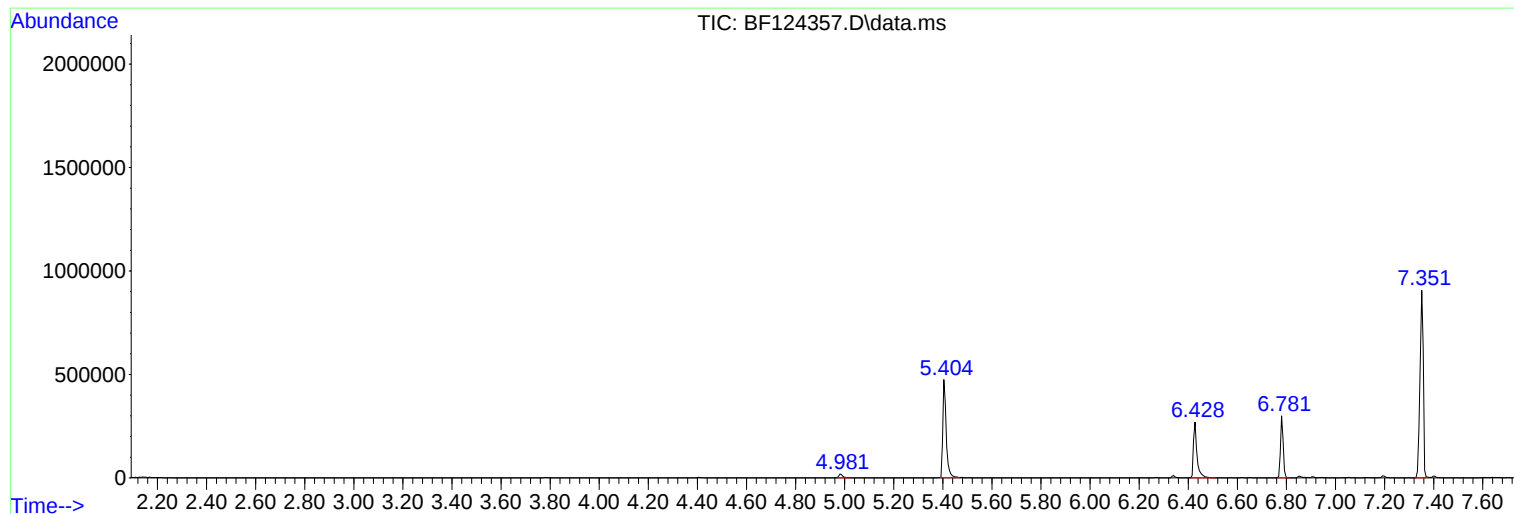
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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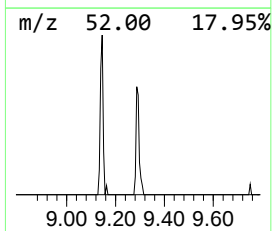
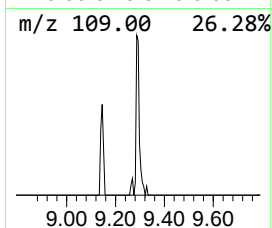
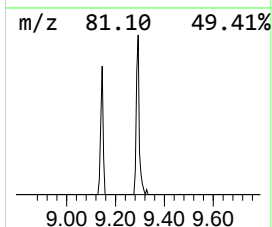
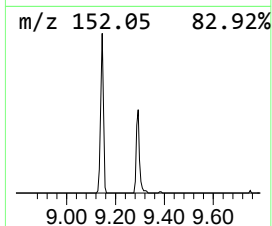
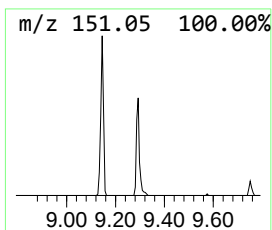
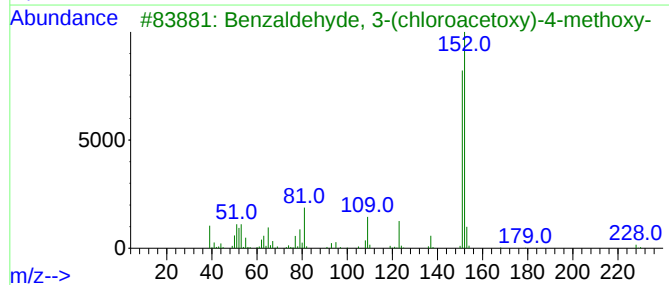
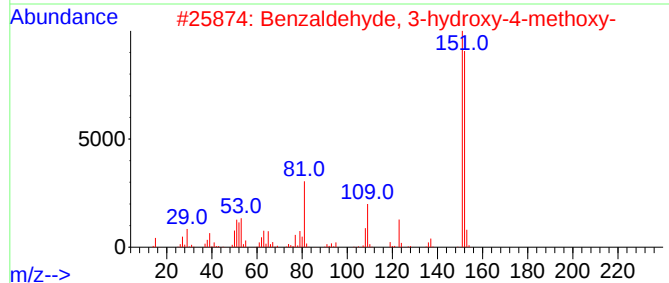
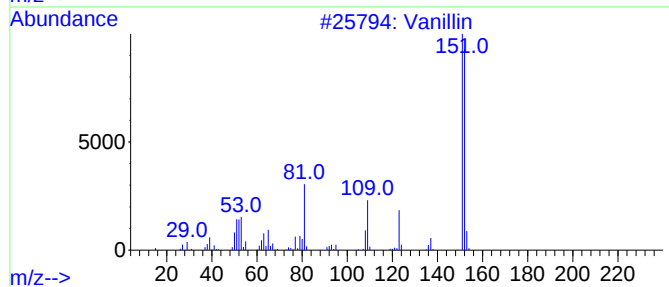
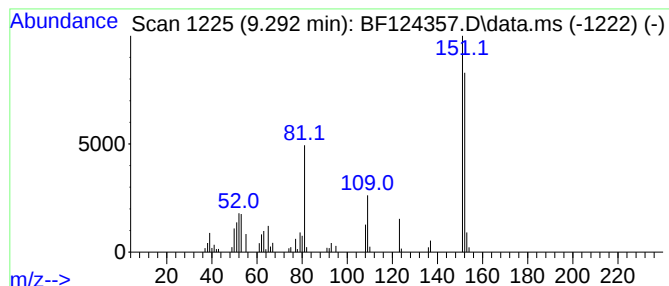
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	6.08 ng	111293	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	96
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	87
3			Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	72
4			Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	72
5			Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	58



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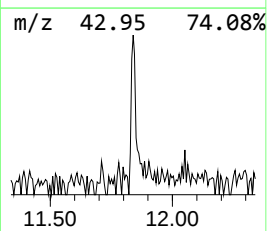
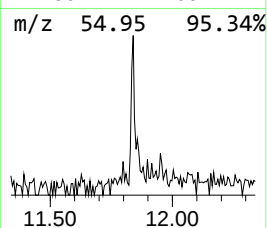
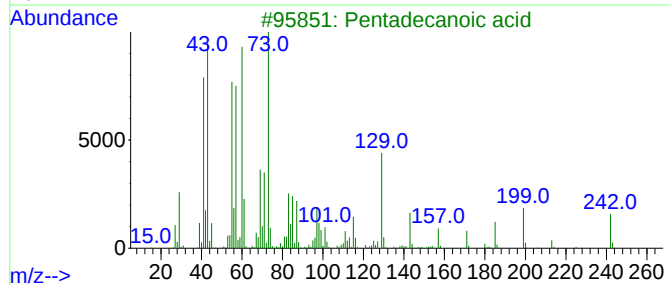
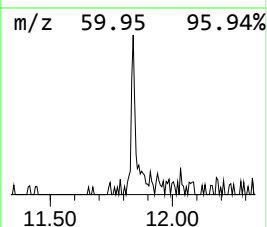
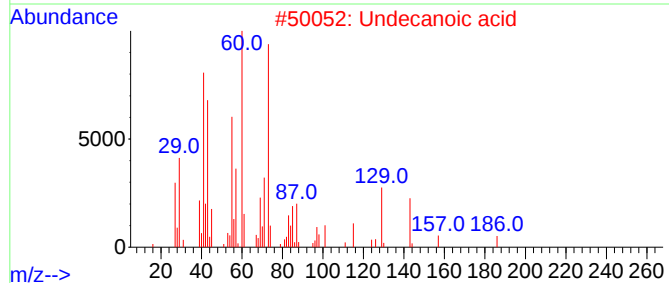
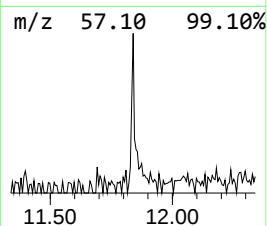
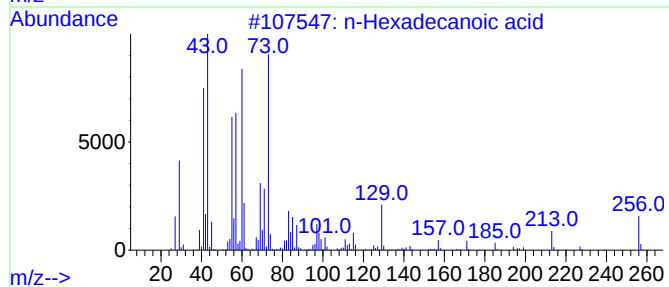
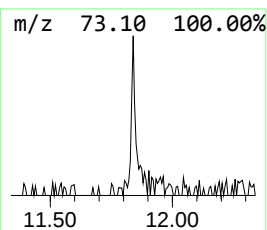
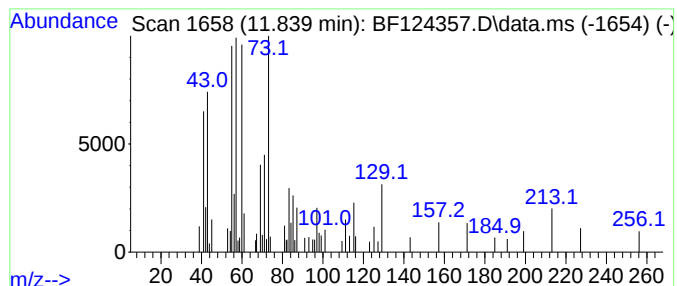
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.25 ng	85975	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Undecanoic acid	186	C11H22O2	000112-37-8	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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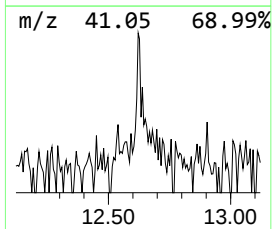
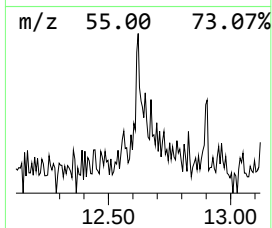
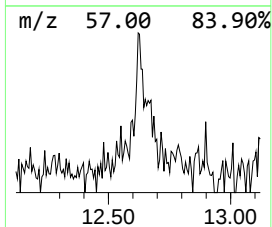
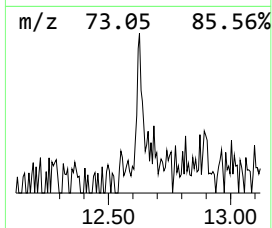
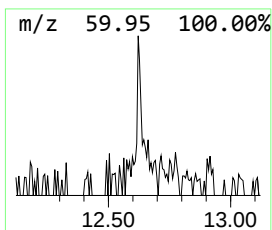
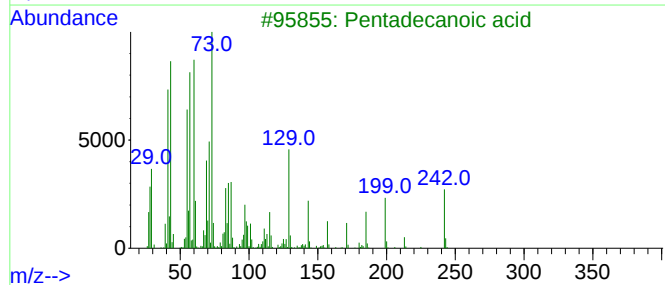
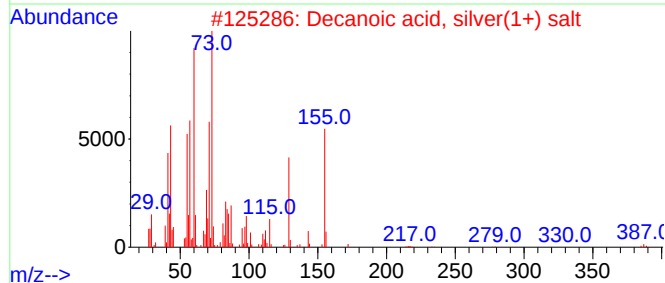
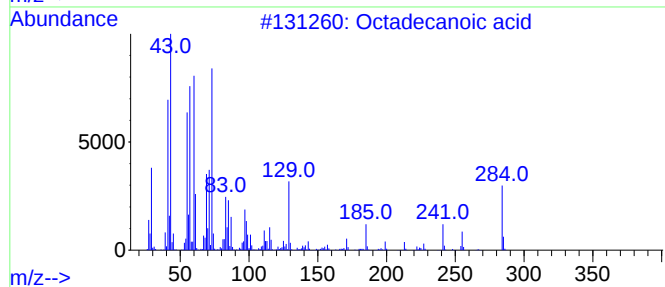
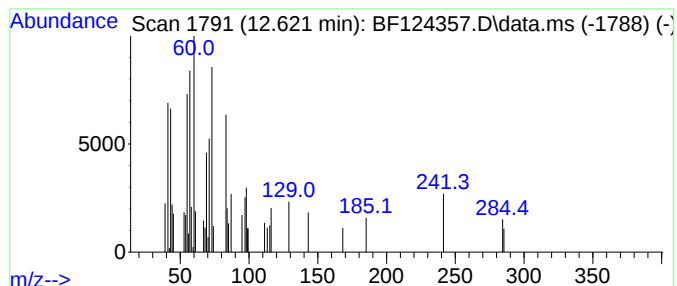
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.621	3.81 ng	77123	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	53
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	37
4			Undecanoic acid	186	C11H22O2	000112-37-8	35
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	32



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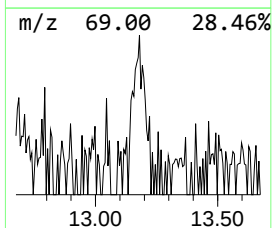
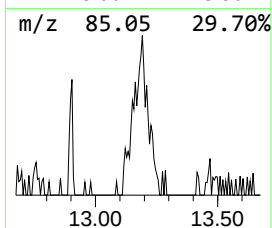
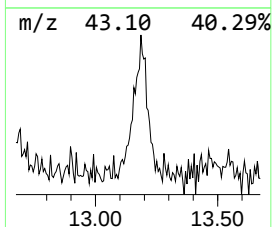
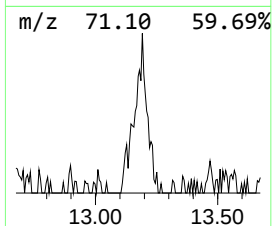
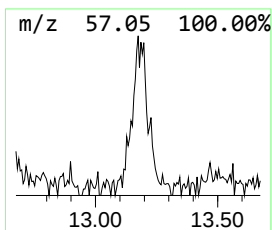
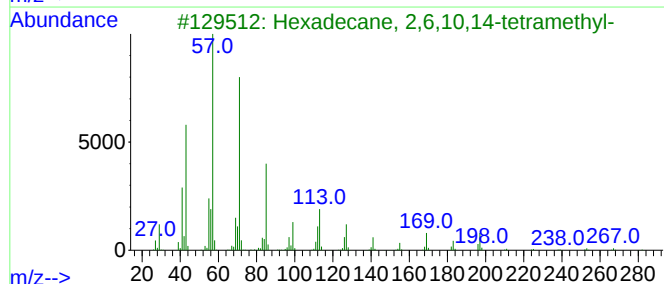
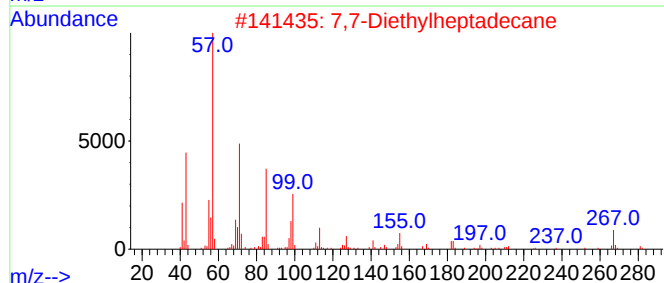
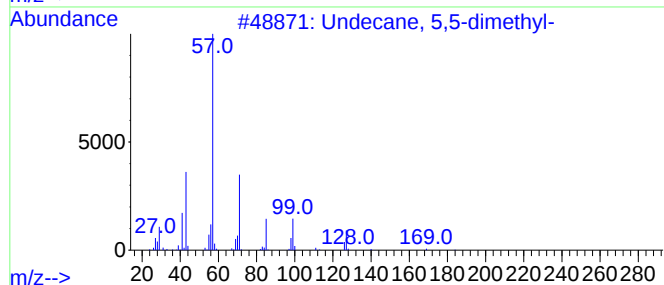
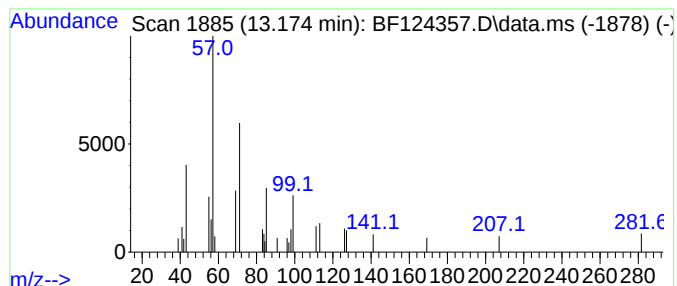
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Peak Number 4 Undecane, 5,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	2.24 ng	38116	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5,5-dimethyl-	184	C13H28	017312-73-1	59
2			7,7-Diethylheptadecane	296	C21H44	1000360-41-5	59
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	53
4			Heptacosane	380	C27H56	000593-49-7	50
5			Tetradecane, 2-methyl-	212	C15H32	001560-95-8	47



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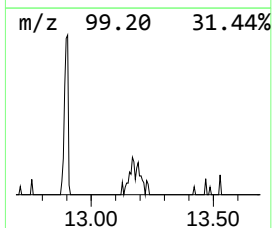
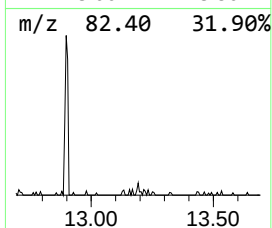
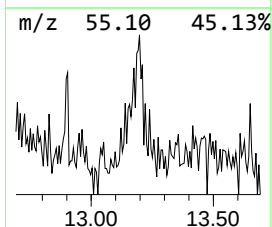
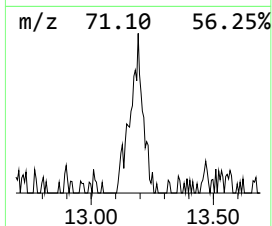
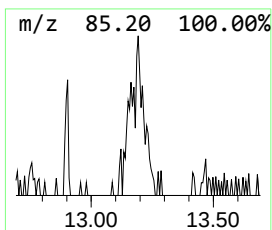
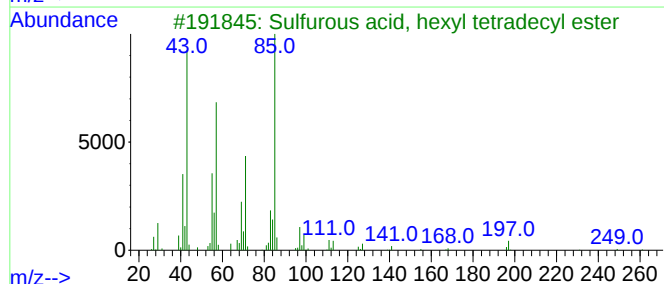
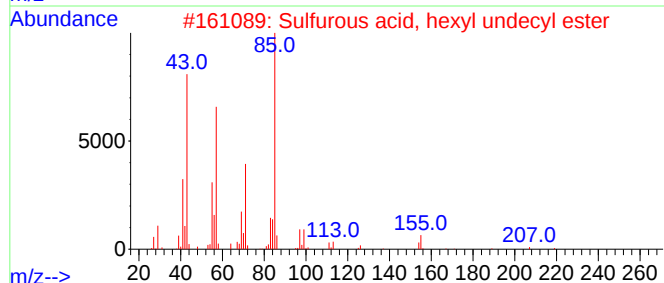
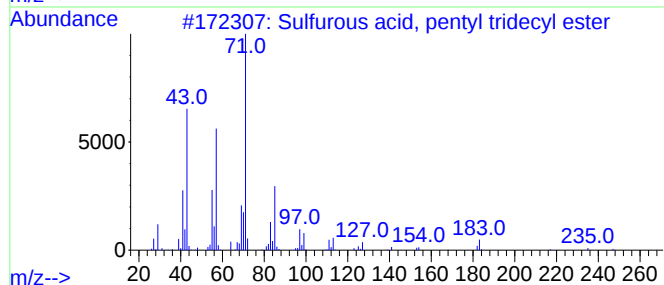
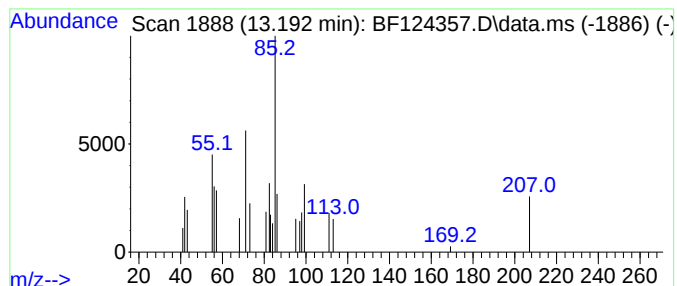
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown13.192 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	3.58 ng	60789	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, pentyl tridecyl ...	334	C18H38O3S	1000309-14-6	32
2			Sulfurous acid, hexyl undecyl ester	320	C17H36O3S	1000309-13-3	28
3			Sulfurous acid, hexyl tetradecyl...	362	C20H42O3S	1000309-13-6	28
4			Valeric acid, 2-tetradecyl ester	298	C19H38O2	055193-14-1	25
5			Octan-2-yl 2-methylbutanoate	214	C13H26O2	1000372-74-3	25



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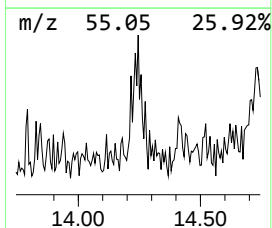
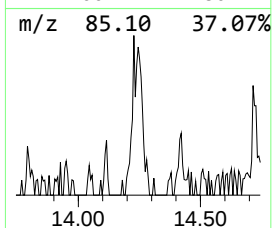
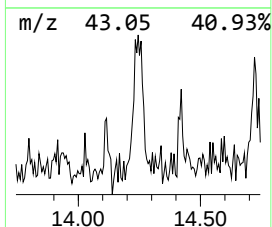
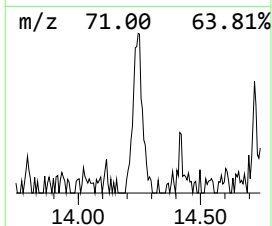
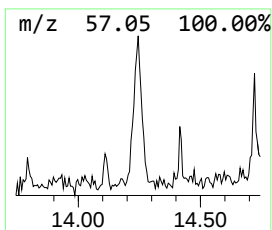
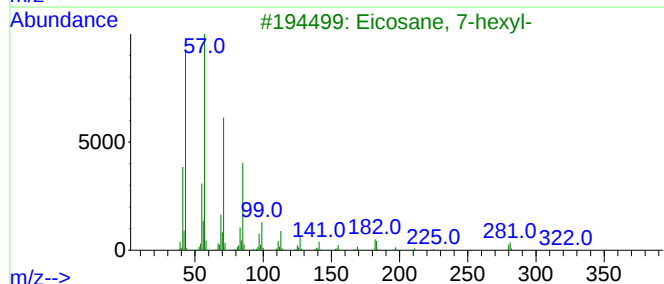
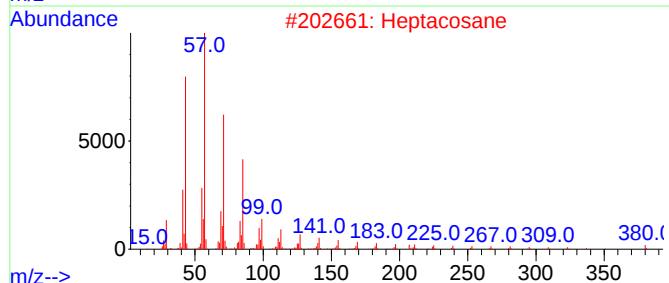
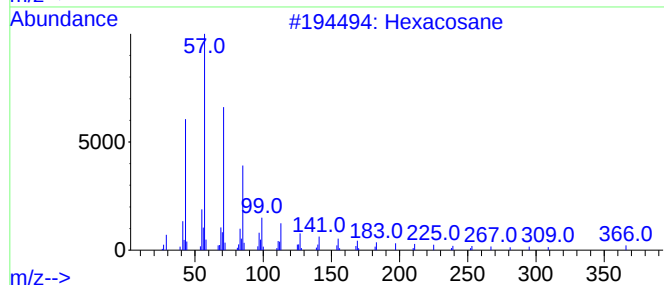
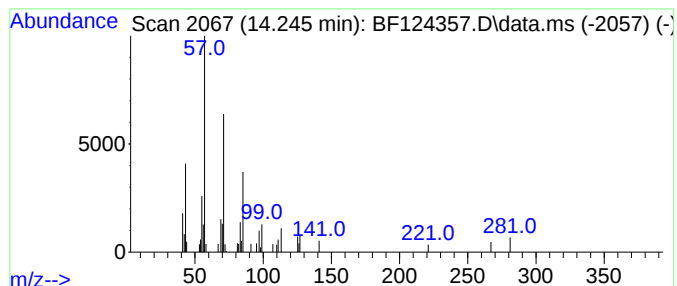
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	6.15 ng	104489	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061721\
Data File : BF124357.D
Acq On : 17 Jun 2021 11:38
Operator : JU/CG
Sample : M2678-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPLP-AMND-COMP-D(CL-01A)

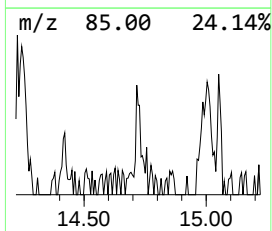
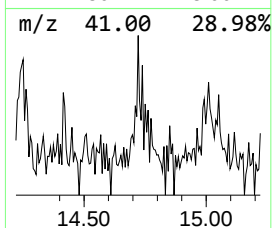
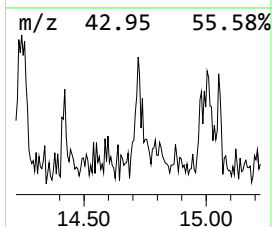
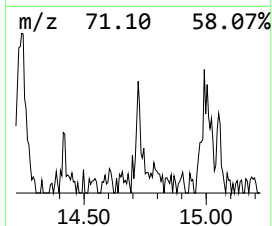
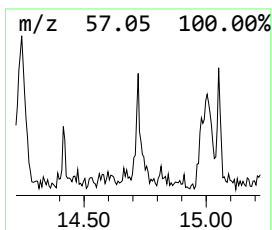
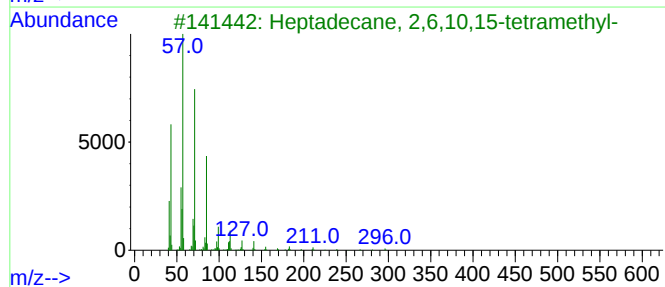
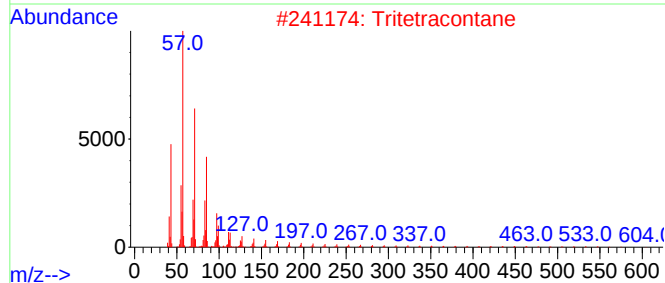
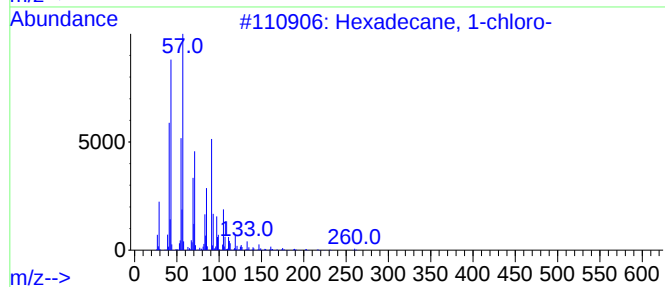
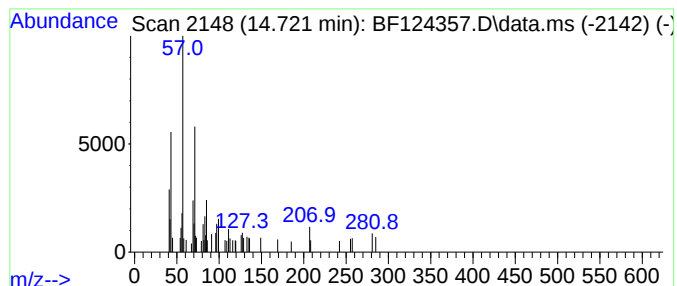
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane, 1-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.52 ng	43402	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	64
2			Tritetracontane	605	C43H88	007098-21-7	53
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	50
4			Hexatriacontane	507	C36H74	000630-06-8	50
5			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061721\
Data File : BF124357.D
Acq On : 17 Jun 2021 11:38
Operator : JU/CG
Sample : M2678-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPLP-AMND-COMP-D(CL-01A)

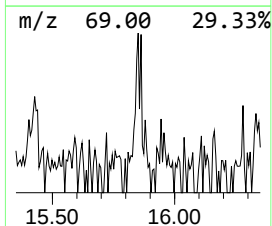
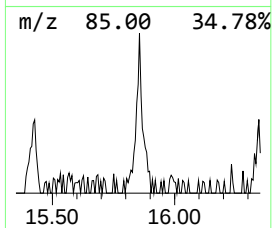
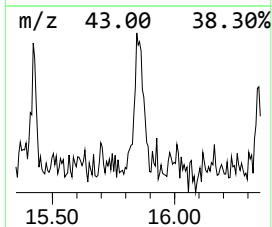
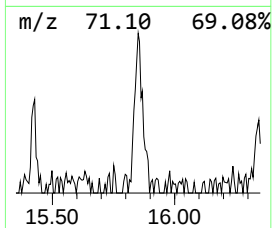
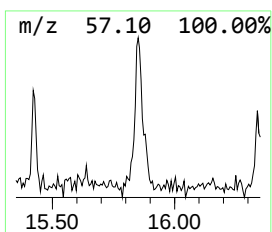
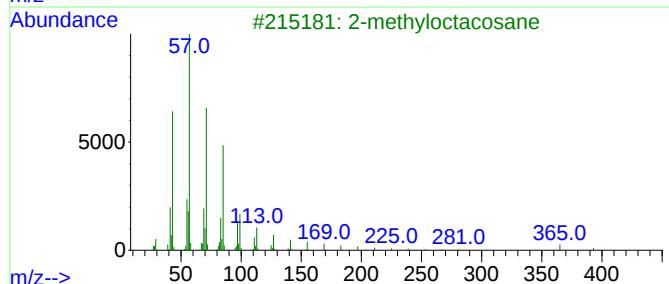
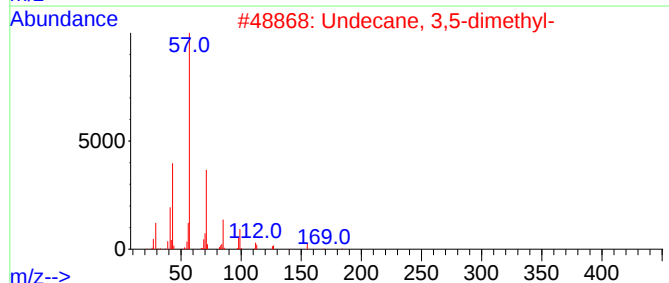
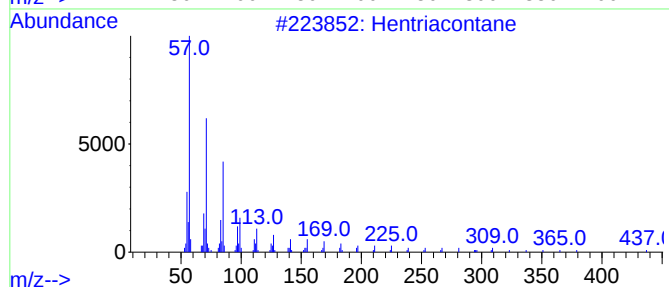
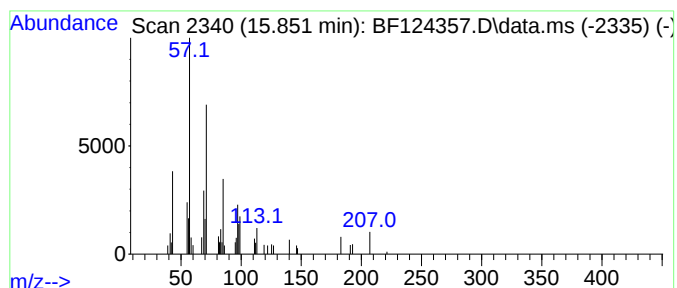
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	5.25 ng	90424	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	59
2			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	58
3			2-methyloctacosane	408	C29H60	1000376-72-8	53
4			Hexacosane	366	C26H54	000630-01-3	53
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061721\
Data File : BF124357.D
Acq On : 17 Jun 2021 11:38
Operator : JU/CG
Sample : M2678-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPLP-AMND-COMP-D(CL-01A)

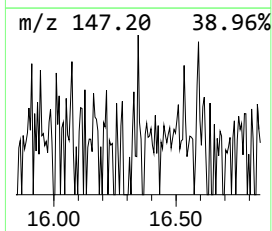
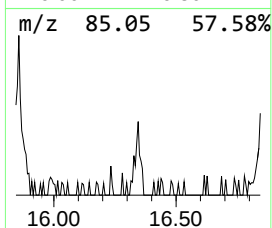
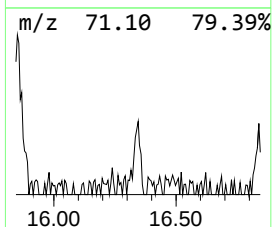
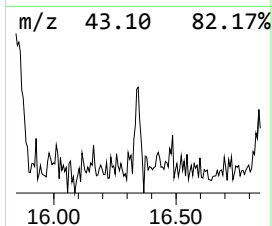
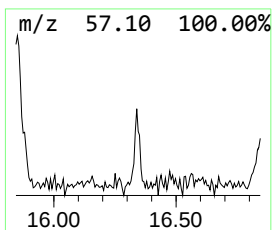
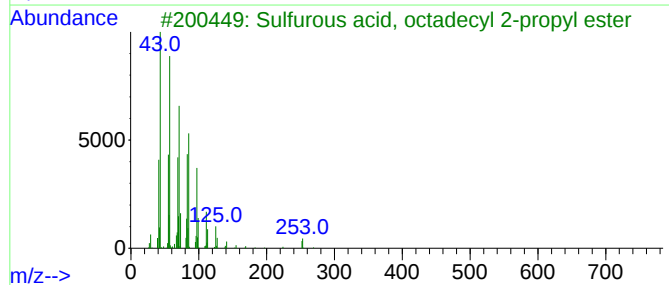
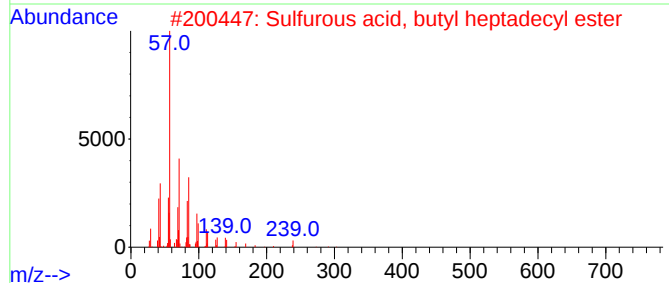
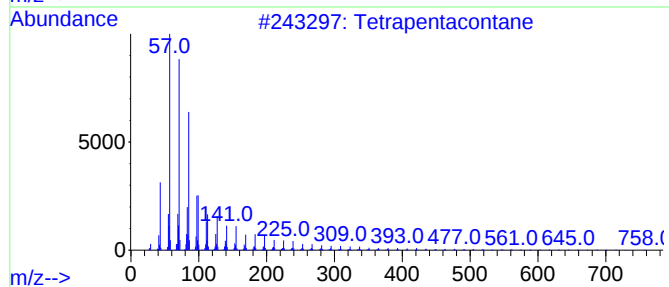
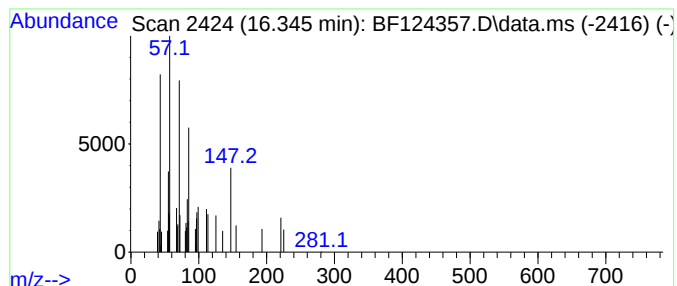
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetrapentacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.345	2.40 ng	41316	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrapentacontane	759	C54H110	005856-66-6	53
2			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	53
3			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	50
4			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	47
5			1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061721\
Data File : BF124357.D
Acq On : 17 Jun 2021 11:38
Operator : JU/CG
Sample : M2678-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPLP-AMND-COMP-D(CL-01A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Vanillin	9.292	6.1	ng	111293	3	9.822	366258	20.0
n-Hexadecanoic ...	11.839	4.3	ng	85975	4	11.310	404328	20.0
Octadecanoic acid	12.621	3.8	ng	77123	4	11.310	404328	20.0
Undecane, 5,5-d...	13.174	2.2	ng	38116	5	13.957	339970	20.0
unknown13.192	13.192	3.6	ng	60789	5	13.957	339970	20.0
Hexacosane	14.245	6.2	ng	104489	5	13.957	339970	20.0
Hexadecane, 1-c...	14.721	2.5	ng	43402	6	15.415	344367	20.0
Hentriacontane	15.851	5.3	ng	90424	6	15.415	344367	20.0
Tetrapentacontane	16.345	2.4	ng	41316	6	15.415	344367	20.0