

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
 Data File : BF126110.D
 Acq On : 10 Nov 2021 16:35
 Operator : JU/CG
 Sample : M4562-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-1

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	13	21	rBV	1244828	1609858	41.24%	5.242%
2	3.940	311	315	320	rVB	54374	64405	1.65%	0.210%
3	5.475	571	576	579	rBV	4280259	3836014	98.27%	12.490%
4	6.481	742	747	750	rBV	3827304	3903361	100.00%	12.710%
5	6.851	807	810	814	rBV	1228832	1005435	25.76%	3.274%
6	7.416	897	906	909	rBV	2673151	2448871	62.74%	7.974%
7	8.039	1008	1012	1024	rBV	1291026	1183319	30.32%	3.853%
8	8.133	1024	1028	1032	rVV	1404798	1150090	29.46%	3.745%
9	9.210	1206	1211	1214	rBV	4659883	3708987	95.02%	12.077%
10	9.886	1322	1326	1335	rBV	1422072	1161259	29.75%	3.781%
11	10.674	1456	1460	1471	rVB	2550922	2226012	57.03%	7.248%
12	11.369	1575	1578	1581	rBV	1139055	1004457	25.73%	3.271%
13	11.392	1581	1582	1586	rVV	90684	77850	1.99%	0.253%
14	11.427	1586	1588	1594	rVB4	33736	48923	1.25%	0.159%
15	11.768	1642	1646	1649	rVB	88637	71636	1.84%	0.233%
16	12.474	1763	1766	1769	rVB	90645	81036	2.08%	0.264%
17	12.580	1782	1784	1789	rVB	192130	158750	4.07%	0.517%
18	12.627	1789	1792	1796	rBV	83723	70523	1.81%	0.230%
19	12.810	1816	1823	1826	rBV	155639	174150	4.46%	0.567%
20	12.957	1844	1848	1851	rBV	3660795	2884976	73.91%	9.394%
21	13.862	1999	2002	2008	rVB2	230248	276787	7.09%	0.901%
22	14.010	2022	2027	2030	rBV	1142604	1087692	27.87%	3.542%
23	14.033	2030	2031	2034	rVB	90474	53385	1.37%	0.174%
24	14.504	2105	2111	2116	rBV4	151821	301260	7.72%	0.981%
25	14.868	2170	2173	2176	rVB	64548	65925	1.69%	0.215%
26	14.939	2182	2185	2189	rBV3	69796	74264	1.90%	0.242%
27	15.051	2200	2204	2213	rVB	91850	159877	4.10%	0.521%
28	15.133	2215	2218	2221	rVV	219774	220537	5.65%	0.718%
29	15.168	2221	2224	2234	rVB5	90113	164696	4.22%	0.536%
30	15.351	2252	2255	2260	rBV2	53655	80791	2.07%	0.263%
31	15.474	2272	2276	2280	rBV	631434	768442	19.69%	2.502%
32	15.715	2314	2317	2322	rVB4	71710	93352	2.39%	0.304%
33	15.951	2353	2357	2362	rBV	164081	264681	6.78%	0.862%
34	17.556	2625	2630	2637	rBV	87414	230381	5.90%	0.750%

Sum of corrected areas: 30711982

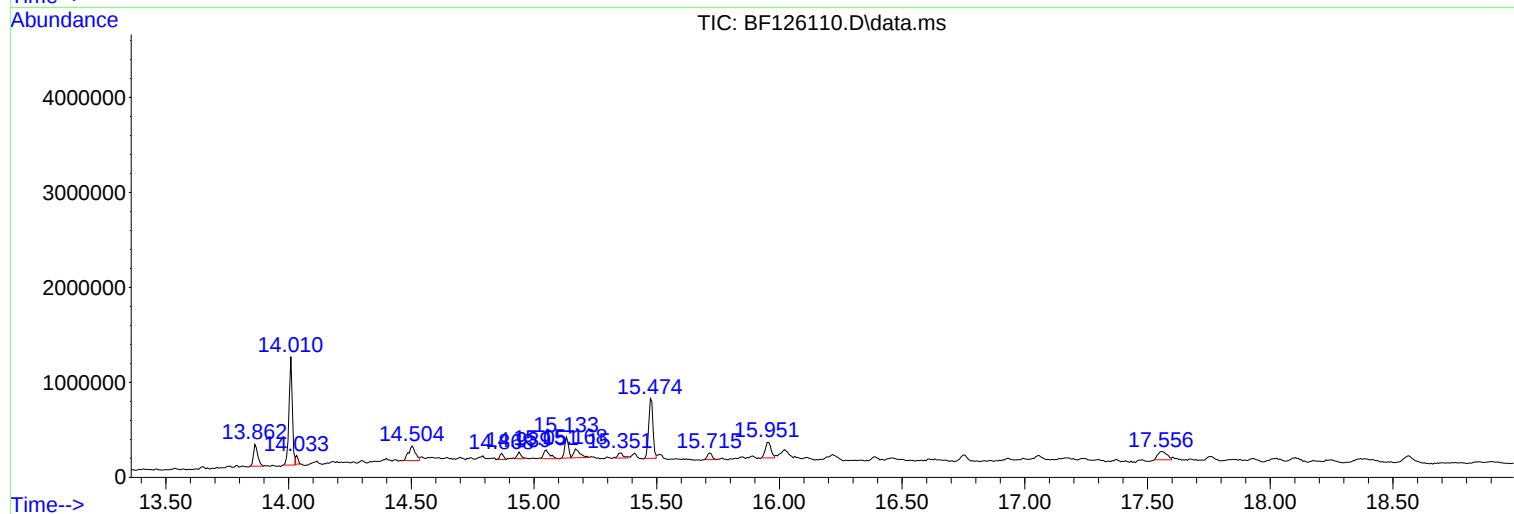
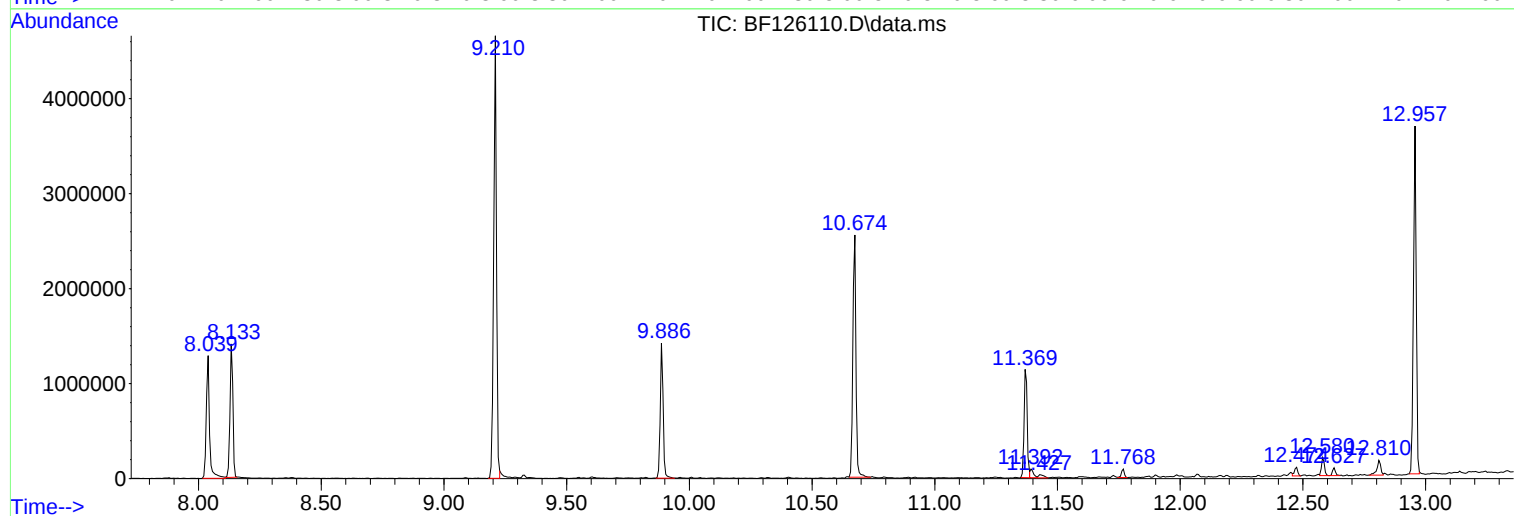
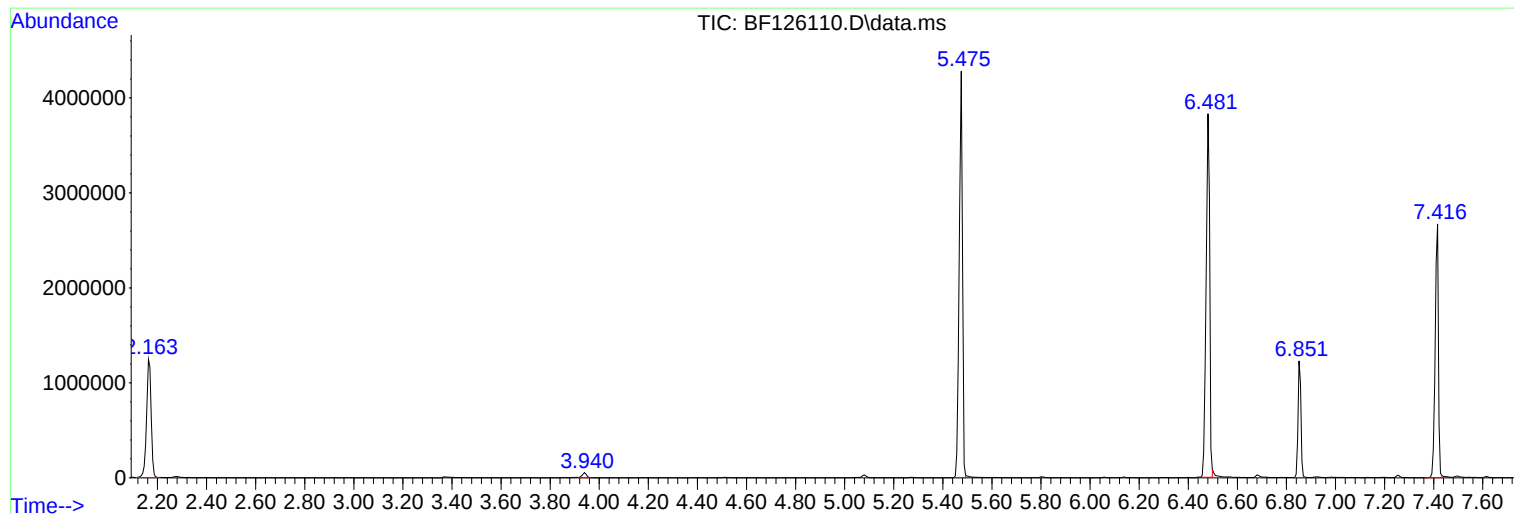
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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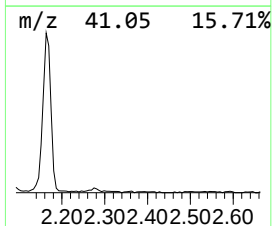
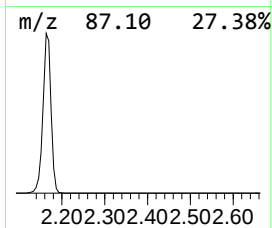
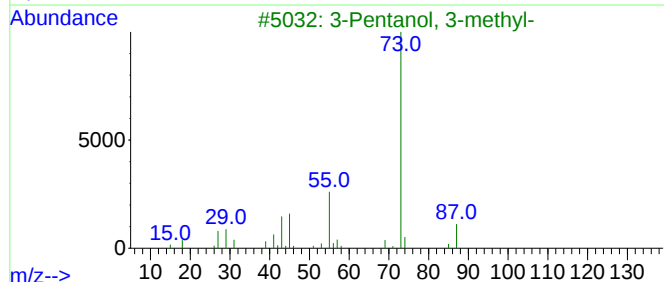
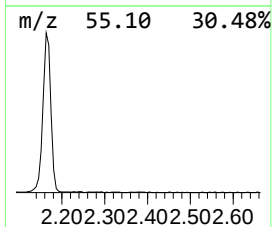
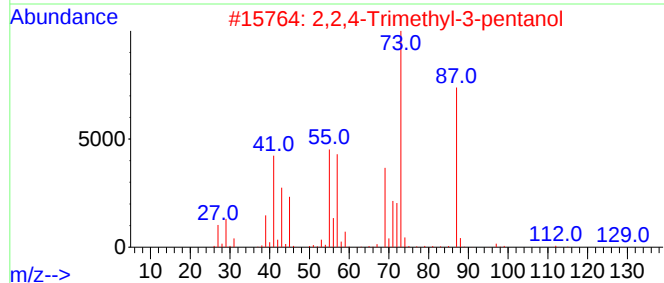
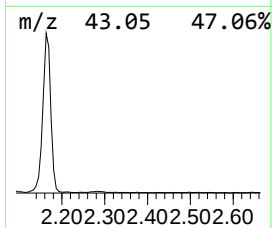
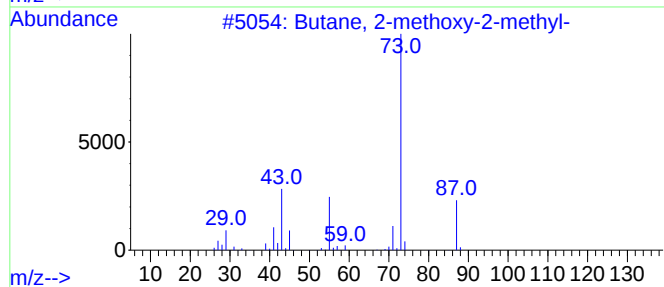
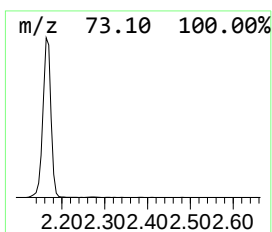
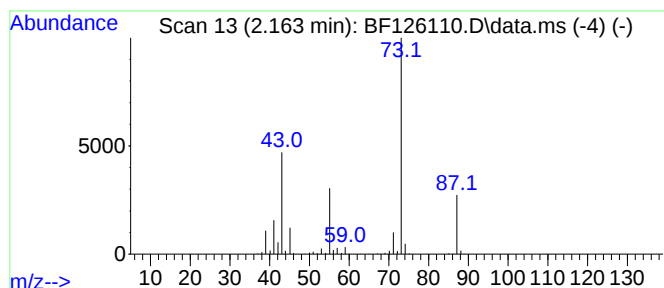
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	32.02 ng	1609860	1,4-Dichlorobenzene-d4	6.851

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	40
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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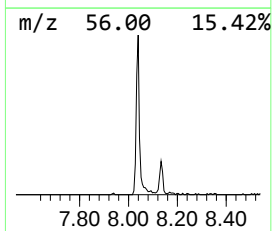
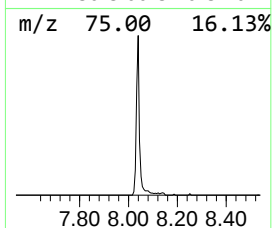
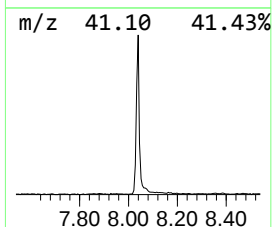
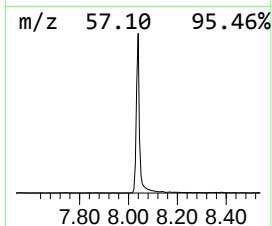
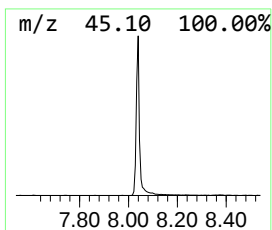
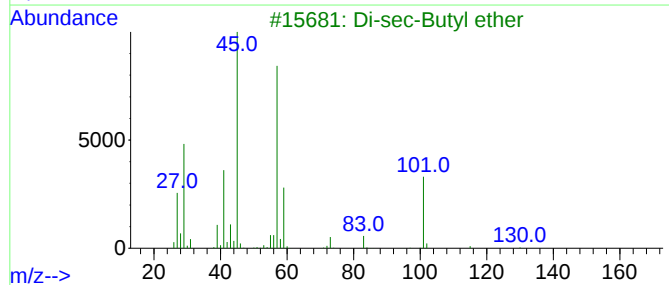
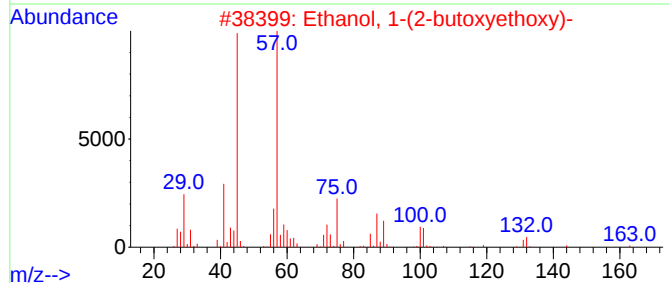
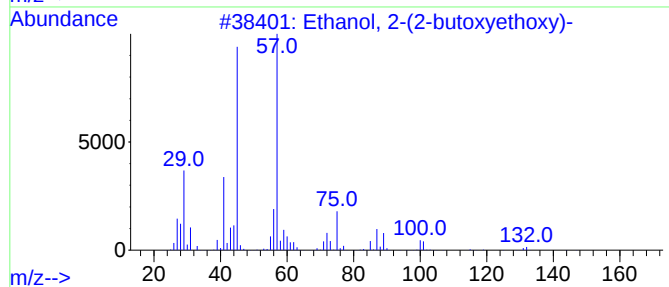
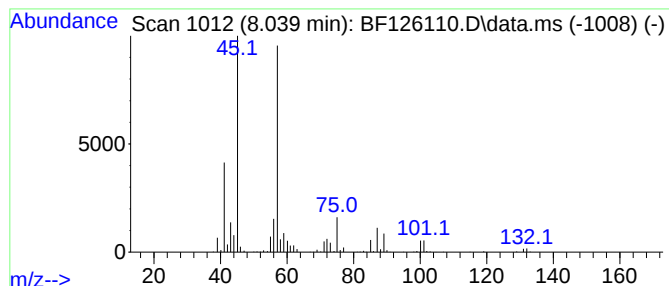
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	20.58 ng	1183320	Naphthalene-d8	8.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Butyl lactate	146	C7H14O3	000138-22-7	50



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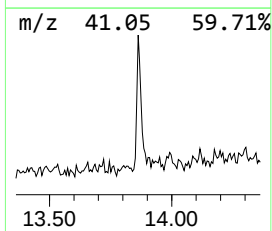
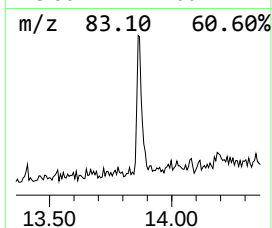
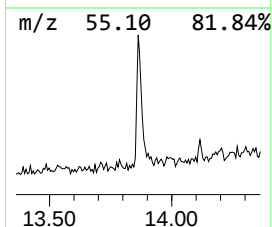
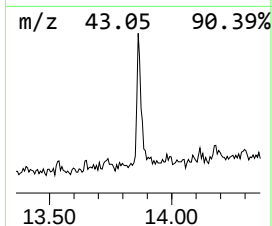
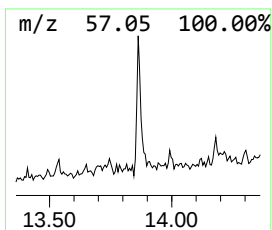
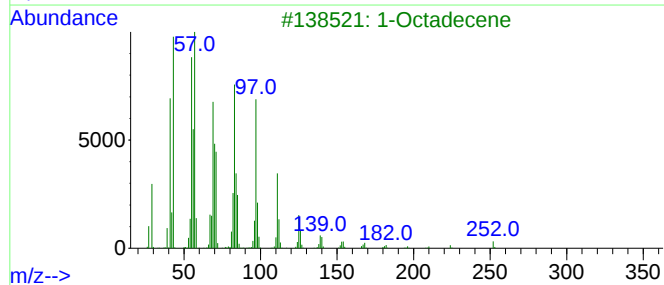
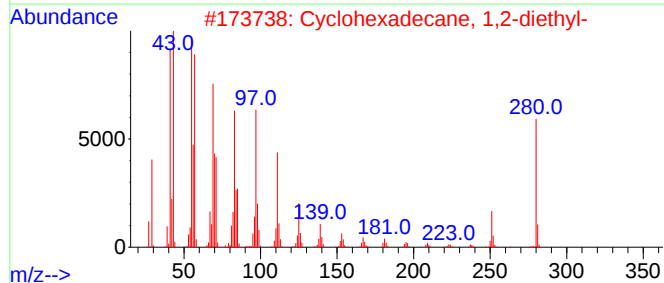
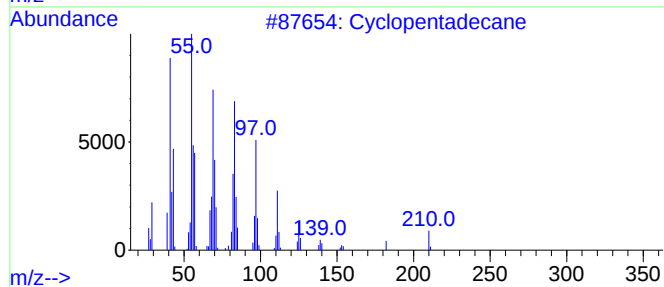
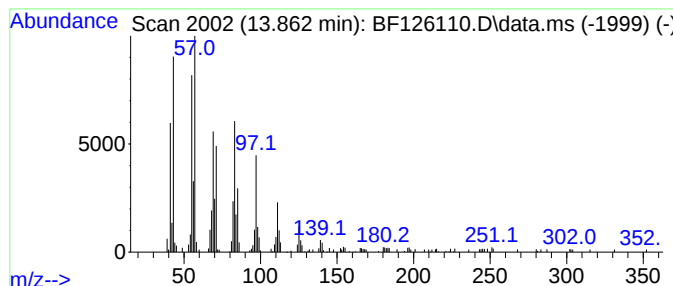
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Peak Number 3 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	5.09 ng	276787	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
3			1-Octadecene	252	C18H36	000112-88-9	95
4			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
5			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94



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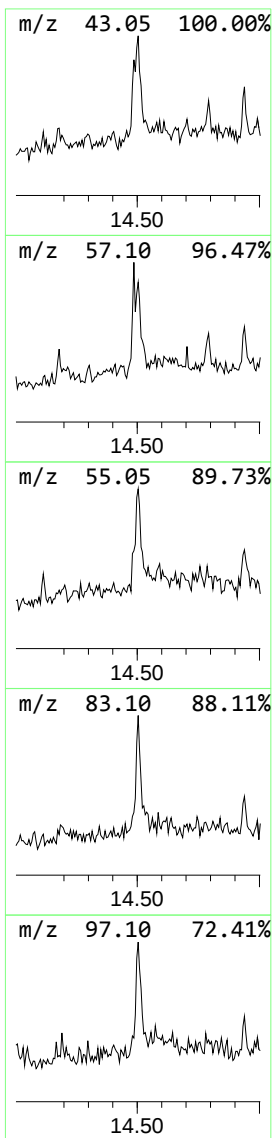
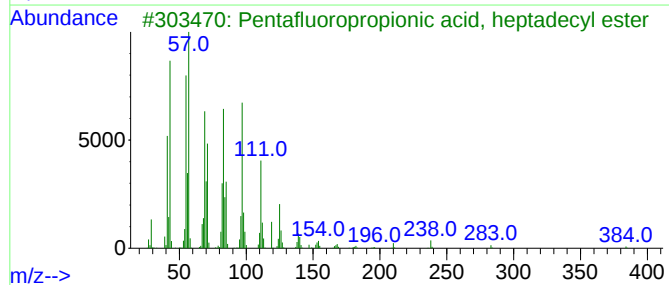
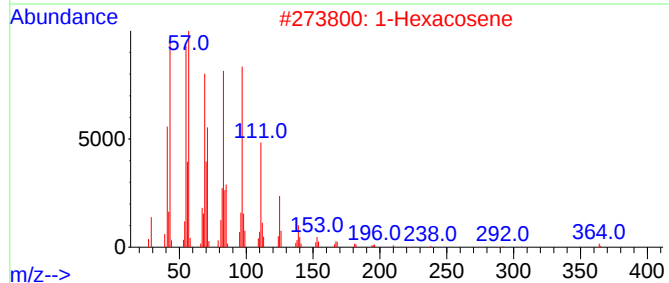
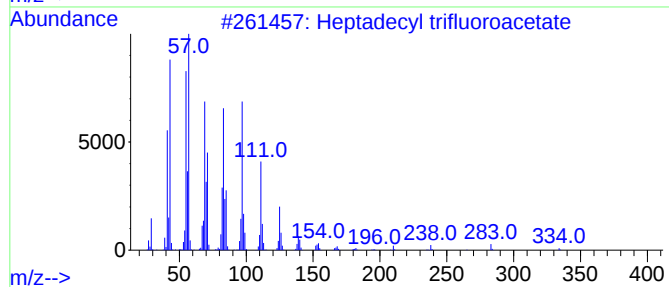
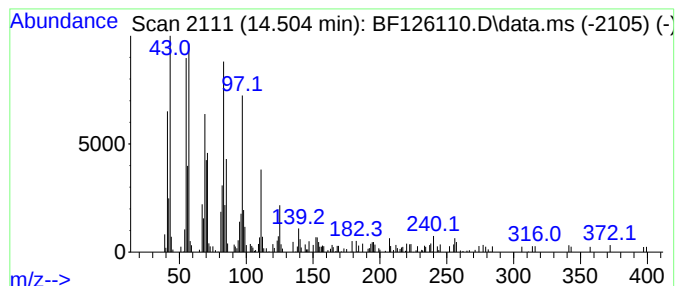
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.504	5.54 ng	301260	Chrysene-d12	14.009	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	89
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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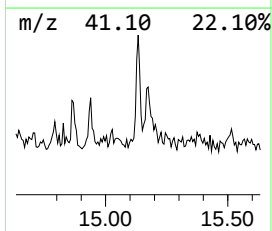
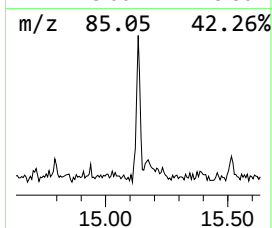
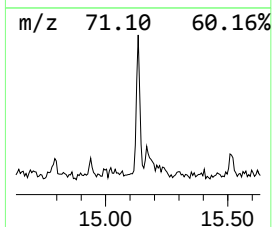
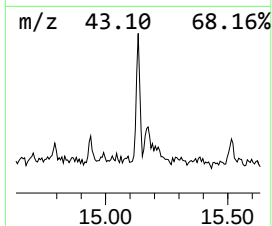
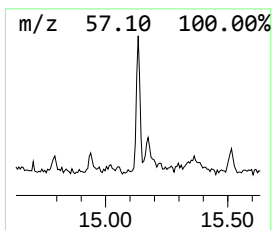
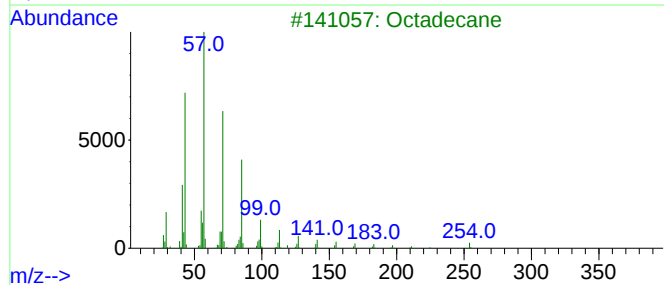
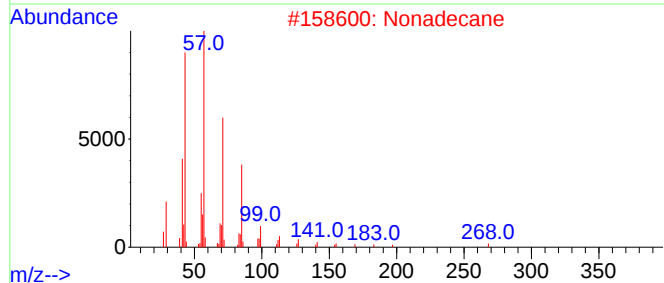
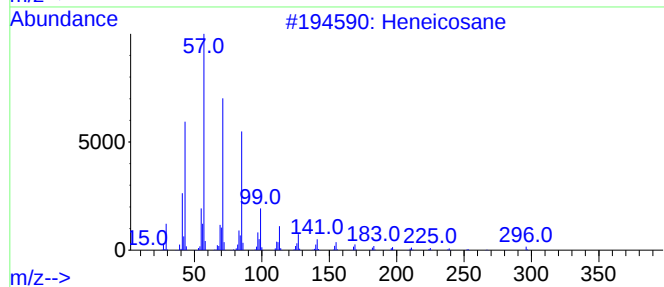
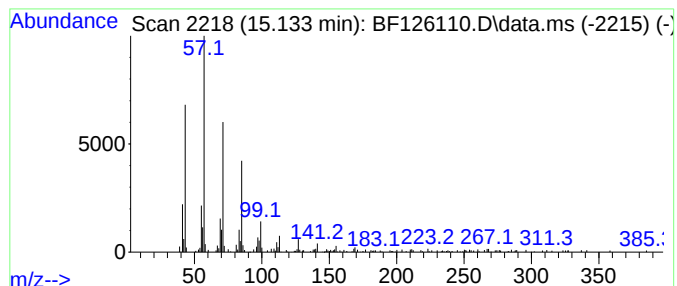
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Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	5.74 ng	220537	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Nonadecane	268	C19H40	000629-92-5	93
3			Octadecane	254	C18H38	000593-45-3	93
4			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
5			Octacosane	394	C28H58	000630-02-4	87



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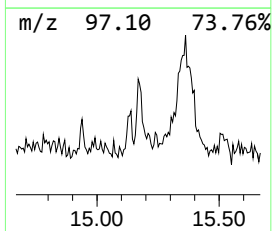
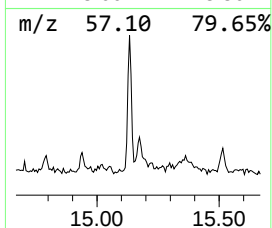
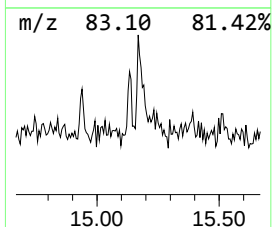
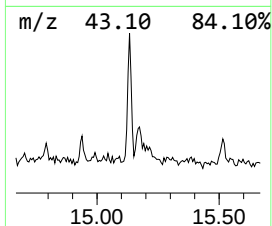
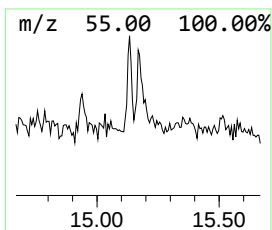
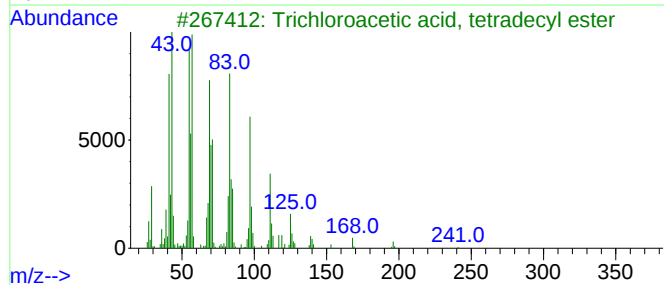
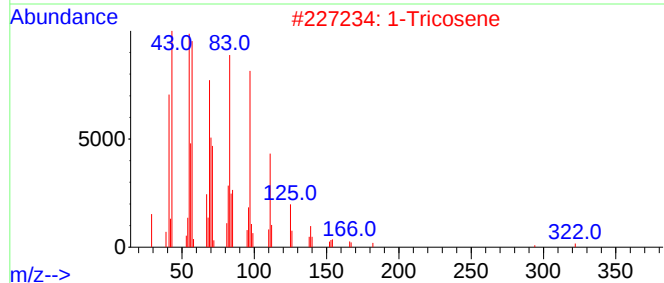
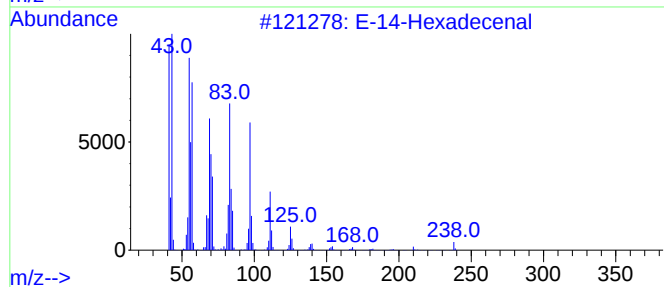
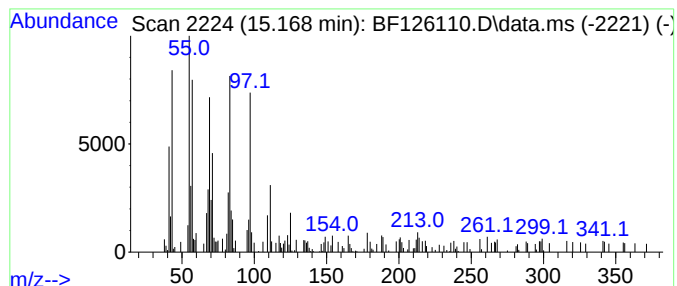
Instrument :
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ClientSampleId :
T-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 E-14-Hexadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.168	4.29 ng	164696	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	90
2	1-Tricosene	322	C23H46	018835-32-0	78
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	72
4	10-Heneicosene (c,t)	294	C21H42	095008-11-0	64
5	1-Nonadecene	266	C19H38	018435-45-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126110.D
Acq On : 10 Nov 2021 16:35
Operator : JU/CG
Sample : M4562-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-1

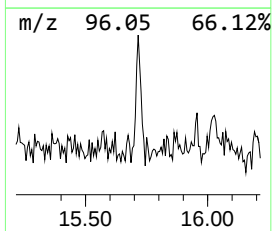
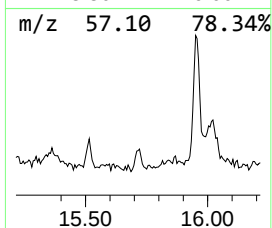
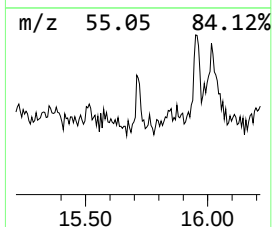
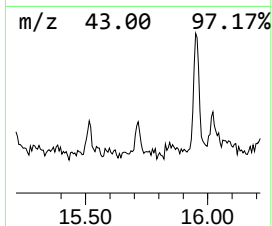
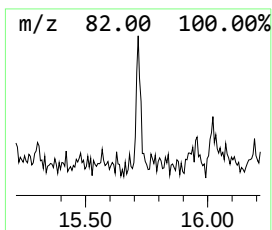
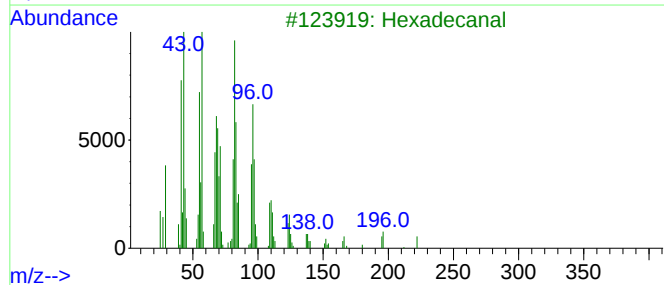
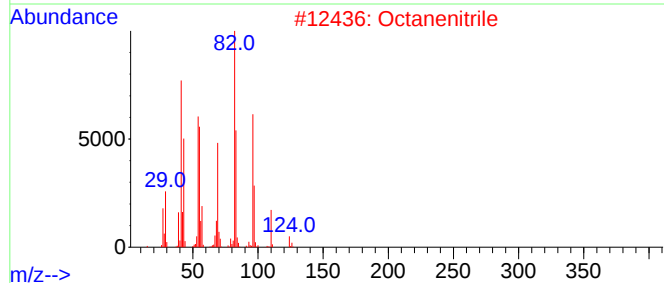
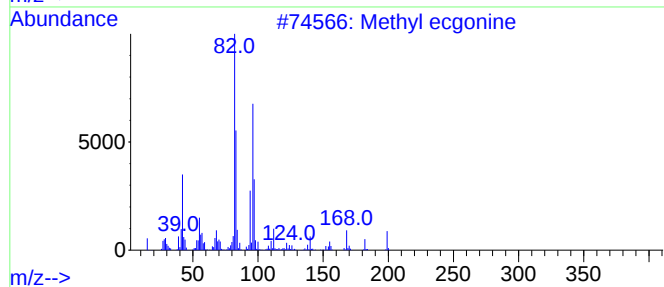
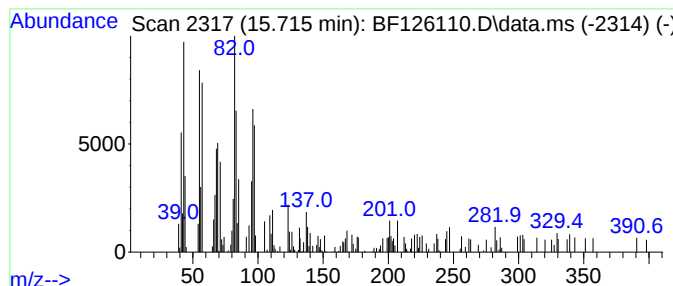
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.715 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	2.43 ng	93352	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ecgonine	199	C10H17NO3	007143-09-1	45
2			Octanenitrile	125	C8H15N	000124-12-9	43
3			Hexadecanal	240	C16H32O	000629-80-1	43
4			9-Undecen-2-one, 6,10-dimethyl-	196	C13H24O	004433-36-7	38
5			1-But-1-enylaziridine	97	C6H11N	1000195-06-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126110.D
Acq On : 10 Nov 2021 16:35
Operator : JU/CG
Sample : M4562-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-1

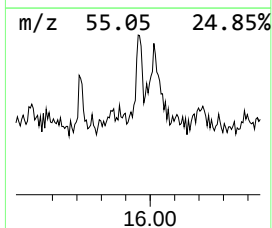
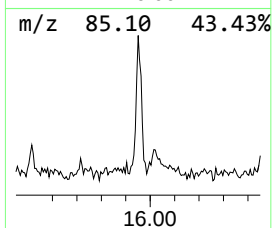
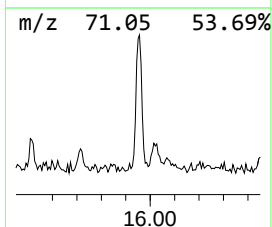
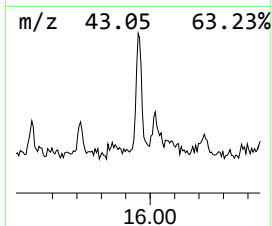
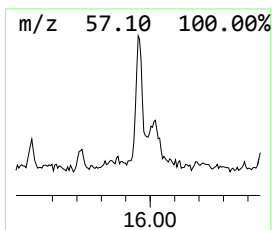
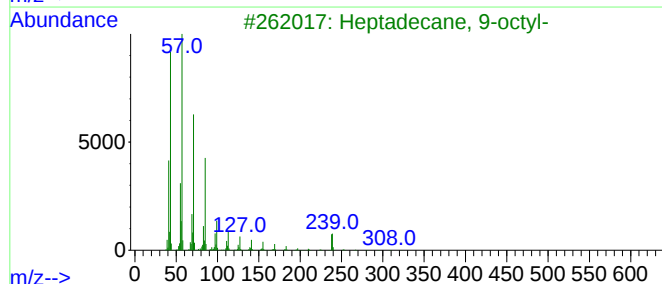
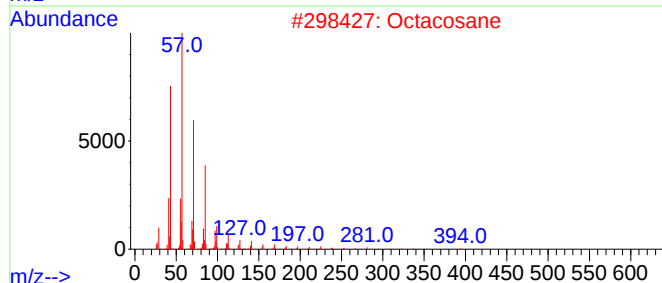
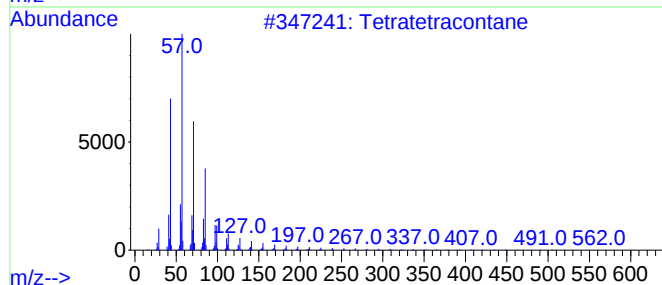
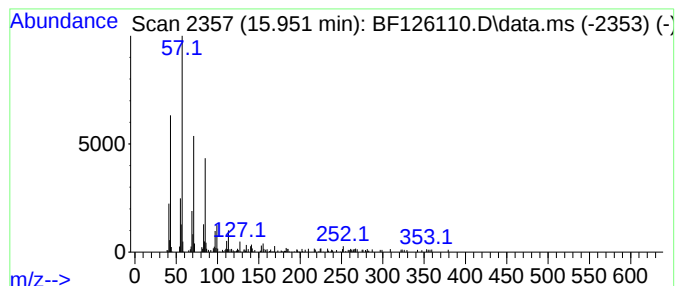
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	6.89 ng	264681	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4			Tetracosane	338	C24H50	000646-31-1	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126110.D
Acq On : 10 Nov 2021 16:35
Operator : JU/CG
Sample : M4562-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

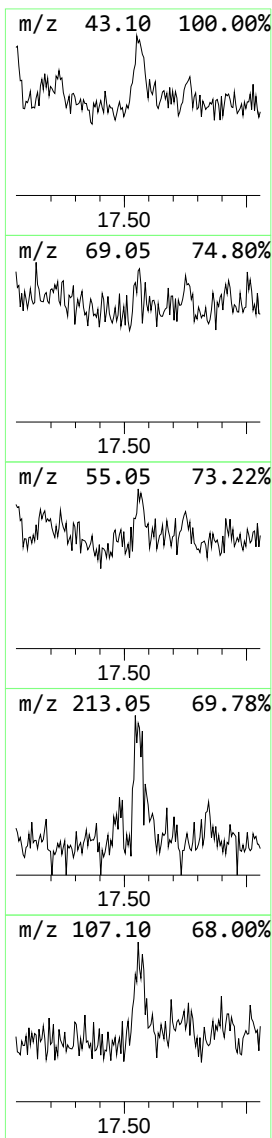
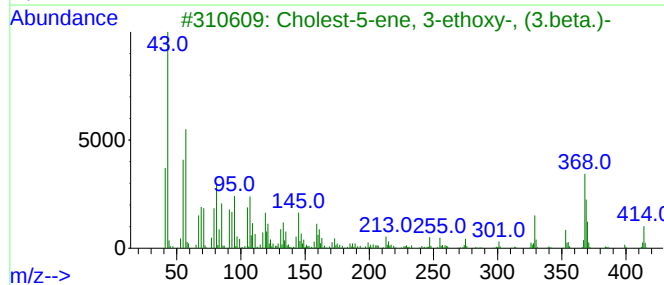
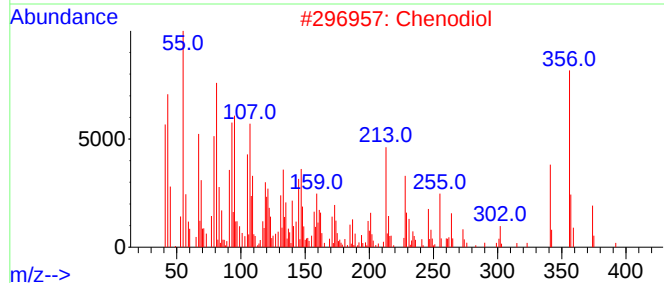
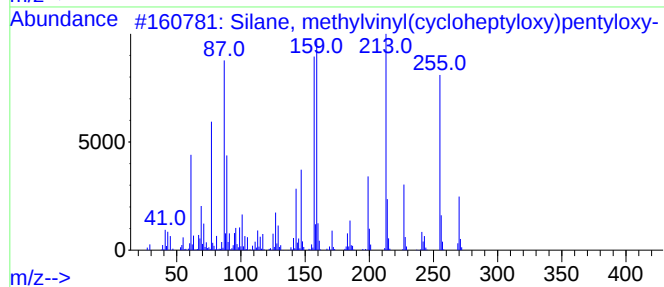
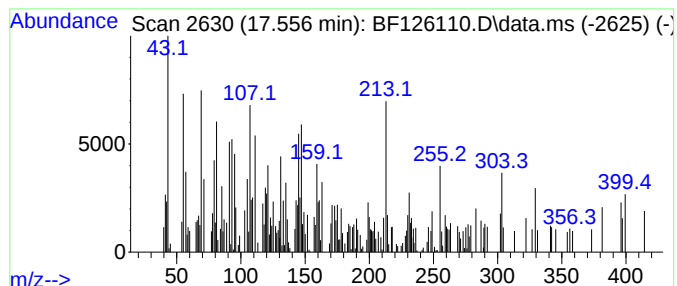
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.556 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.556	6.00 ng	230381	Perylene-d12	15.474
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Silane, methylvinyl(cycloheptylo...	270 C15H3002Si	1000421-02-9 25
2		Chenodiol	392 C24H4004	000474-25-9 13
3		Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H500	000986-19-6 11
4		2H-Indol-2-one, 1,3-dihydro-3-(5...	213 C12H7N03	013191-62-3 11
5		Chola-5,22-dien-3-ol, (3.beta.,2...	342 C24H380	057597-14-5 10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126110.D
Acq On : 10 Nov 2021 16:35
Operator : JU/CG
Sample : M4562-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Butane, 2-metho...	2.163	32.0	ng	1609860	1	6.851	1005440	20.0
Ethanol, 2-(2-b...	8.039	20.6	ng	1183320	2	8.133	1150090	20.0
Cyclopentadecane	13.863	5.1	ng	276787	5	14.009	1087690	20.0
Heptadecyl trif...	14.504	5.5	ng	301260	5	14.009	1087690	20.0
Heneicosane	15.133	5.7	ng	220537	6	15.474	768442	20.0
E-14-Hexadecenal	15.168	4.3	ng	164696	6	15.474	768442	20.0
unknown15.715	15.715	2.4	ng	93352	6	15.474	768442	20.0
Tetratetracontane	15.951	6.9	ng	264681	6	15.474	768442	20.0
unknown17.556	17.556	6.0	ng	230381	6	15.474	768442	20.0