LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072224\
Data File : BF138606.D
Acq On : 22 Jul 2024 14:14
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 285-290

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	5	14	21	rVB	1497633	2350606	92.38%	10.297%
2	3.404	217	223	237	rBV	86881	196213	7.71%	0.860%
3	5.087	504	509	516	rVB	129201	196919	7.74%	0.863%
4	5.487	571	577	588	rBV	1737813	2248205	88.35%	9.848%
5	6.492	742	748	767	rBV	1776961	2438431	95.83%	10.682%
6	6.686	774	781	793	rBV	64395	96795	3.80%	0.424%
7	6.857	805	810	815	rBV	579066	698915	27.47%	3.062%
8	7.422	899	906	911	rBV	1130896	1494960	58.75%	6.549%
9	7.669	943	948	954	rBV	39992	52868	2.08%	0.232%
10	8.139	1022	1028	1033	rBV	661825	817482	32.13%	3.581%
11	8.357	1057	1065	1069	rBV	23164	31345	1.23%	0.137%
12	8.451	1076	1081	1094	rBV	146966	222647	8.75%	0.975%
13	9.216	1204	1211	1216	rBV	1991165	2544517	100.00%	11.146%
14	9.716	1287	1296	1308	rBV4	10652	28555	1.12%	0.125%
15	9.892	1318	1326	1331	rBV	765784	956405	37.59%	4.190%
16	9.992	1335	1343	1355	rBV	1548909	2524269	99.20%	11.058%
17	10.680	1455	1460	1475	rBV	971199	1336220	52.51%	5.853%
18	10.798	1475	1480	1489	rVB3	13287	27280	1.07%	0.119%
19	11.380	1573	1579	1586	rBV	589385	757230	29.76%	3.317%
20	11.763	1639	1644	1649	rBV	21247	28961	1.14%	0.127%
21	11.904	1659	1668	1689	rBV2	181153	346060	13.60%	1.516%
22	12.468	1753	1764	1774	rBV5	30067	82133	3.23%	0.360%
23	12.592	1781	1785	1787	rBV	20589	26157	1.03%	0.115%
24	12.686	1796	1801	1811	rBV	40848	68245	2.68%	0.299%
25	12.963	1842	1848	1853	rBV	1329399	1671698	65.70%	7.323%
26	13.433	1920	1928	1936	rVB	64401	99272	3.90%	0.435%
27	13.868	1995	2002	2015	rBV3	61147	155199	6.10%	0.680%
28	14.015	2022	2027	2040	rVB	402604	566496	22.26%	2.482%
29	14.474	2102	2105	2109	rBV	20611	30450	1.20%	0.133%
30	14.857	2166	2170	2176	rVB2	38674	61686	2.42%	0.270%
31	15.057	2200	2204	2210	rBV	16332	32175	1.26%	0.141%
32	15.121	2211	2215	2219	rVB	42586	58400	2.30%	0.256%
33	15.480	2271	2276	2287	rVB	310544	506067	19.89%	2.217%
34	15.933	2349	2353	2360	rVB	46333	75637	2.97%	0.331%

Sum of corrected areas: 22828498

Instrument :
BNA_F
ClientSampleId :
285-290

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072224\
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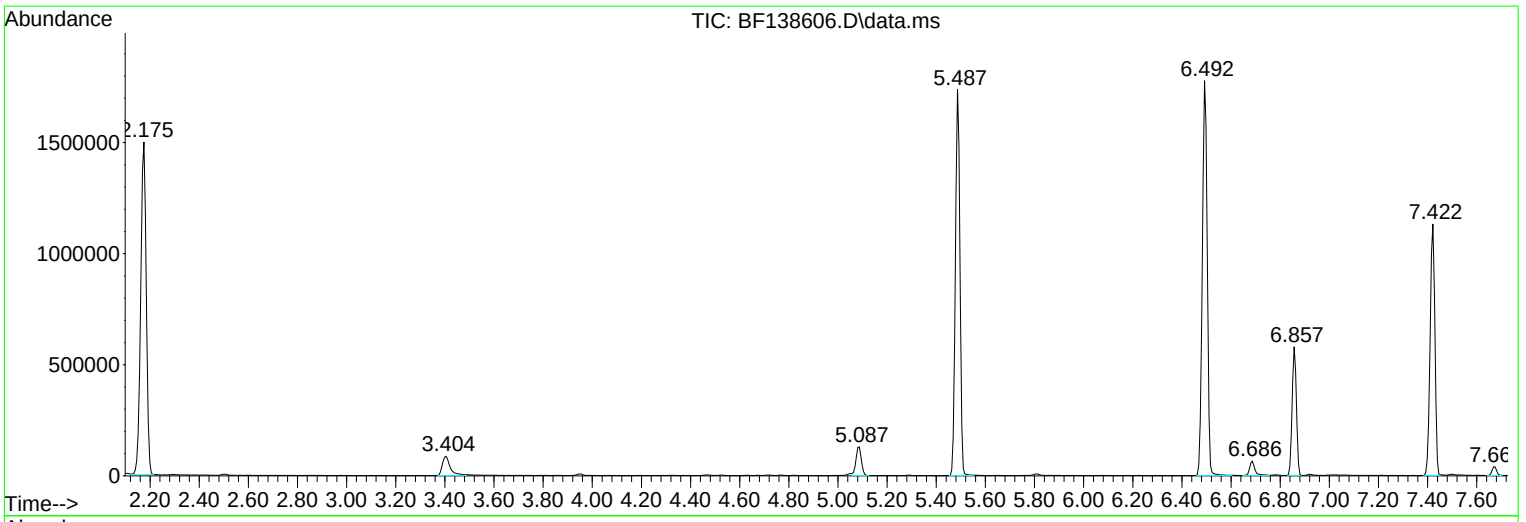
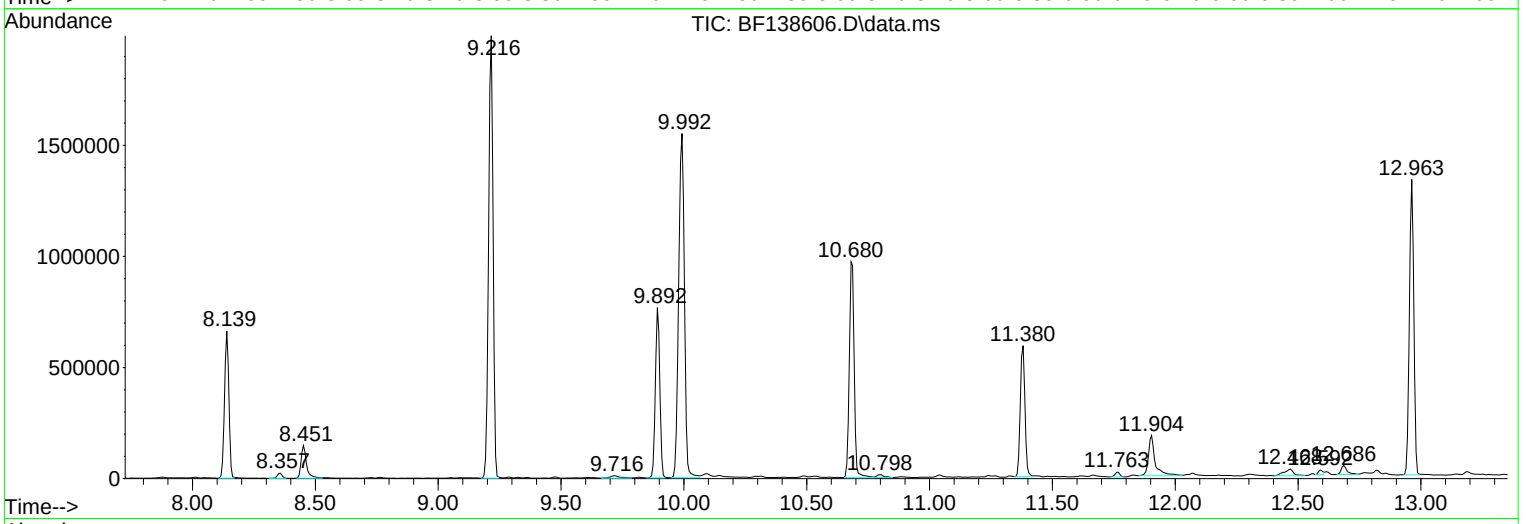
Misc :
ALS Vial : 7 Sample Multiplier: 1

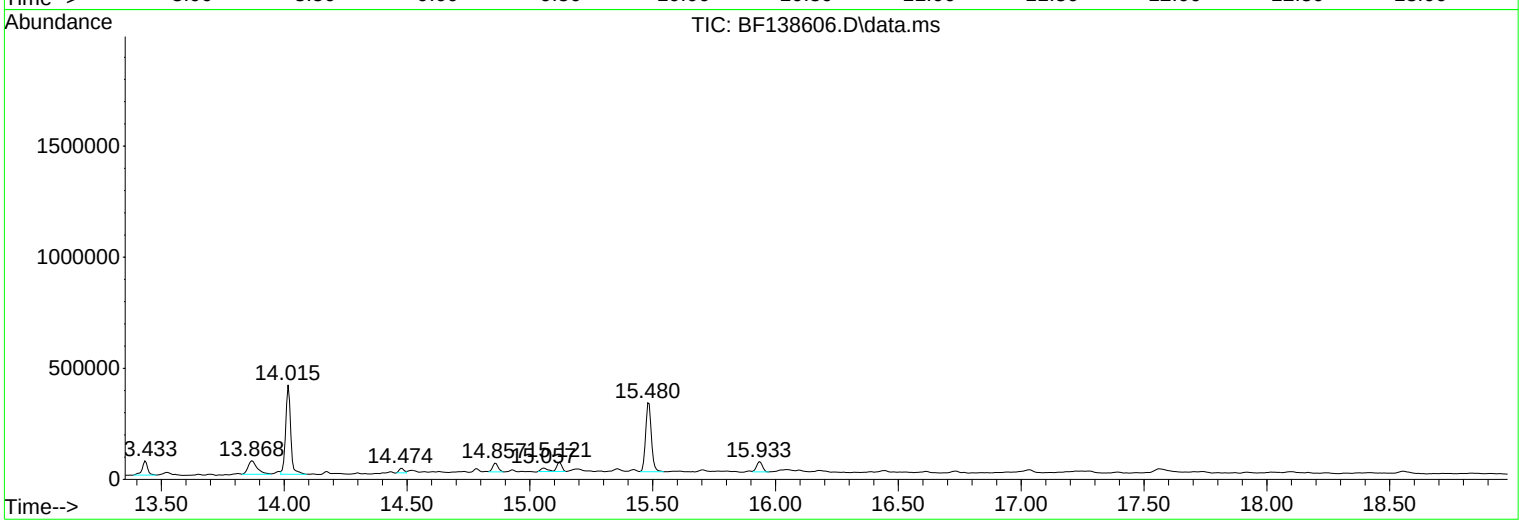
Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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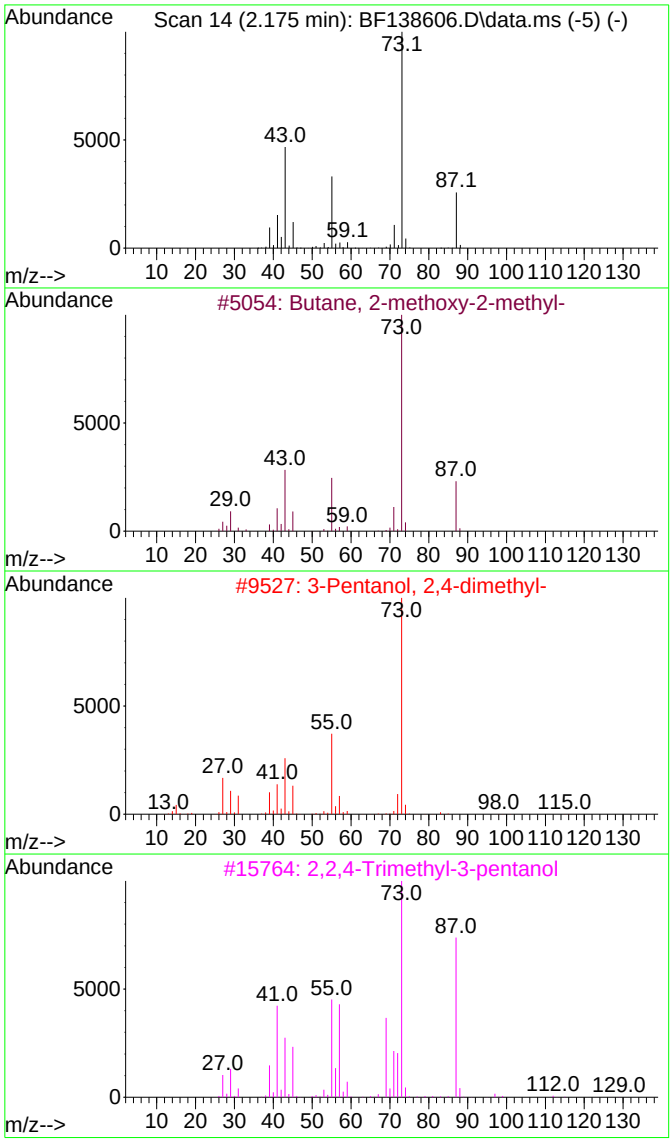
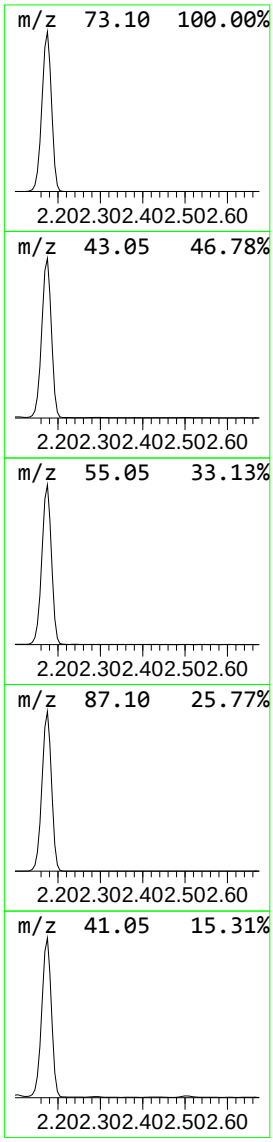
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	67.26 ng	2350610	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
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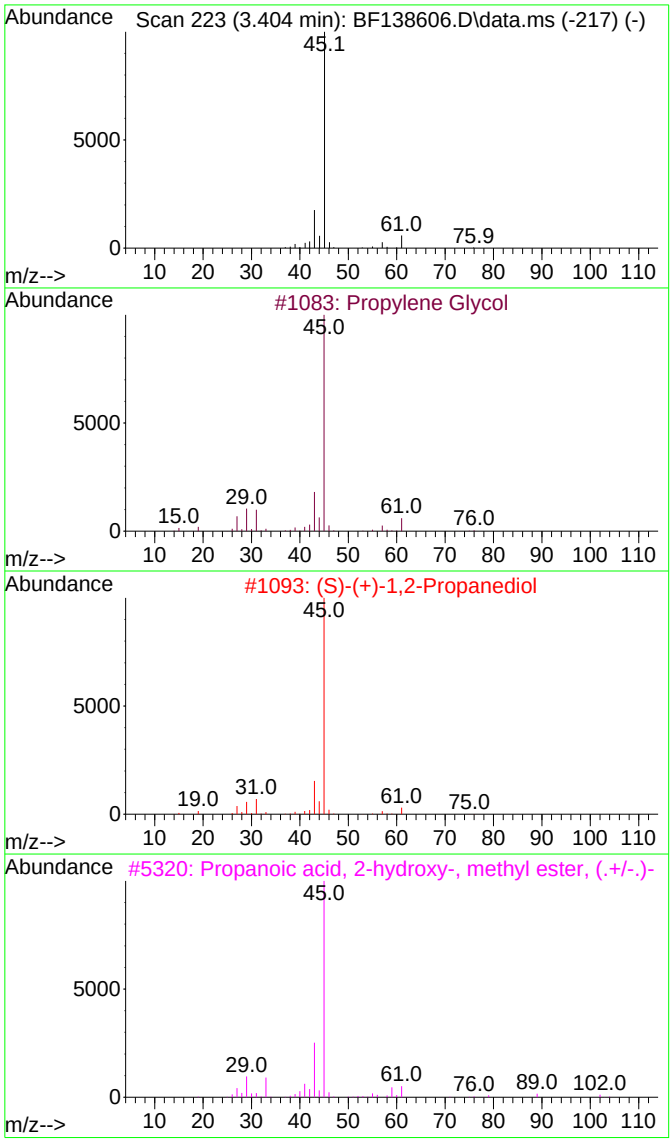
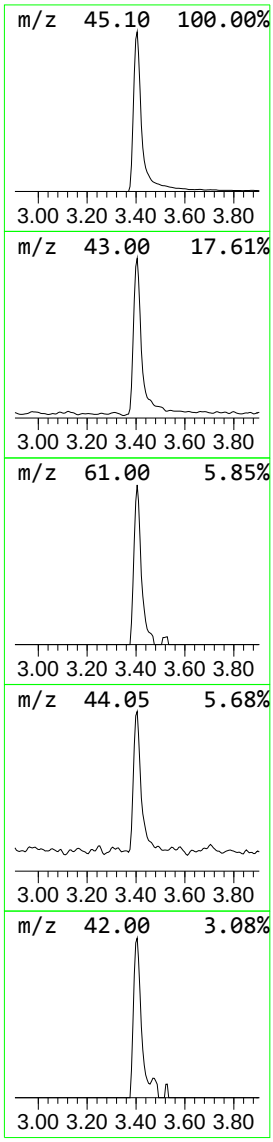
Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	5.61 ng	196213	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	83
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





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Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

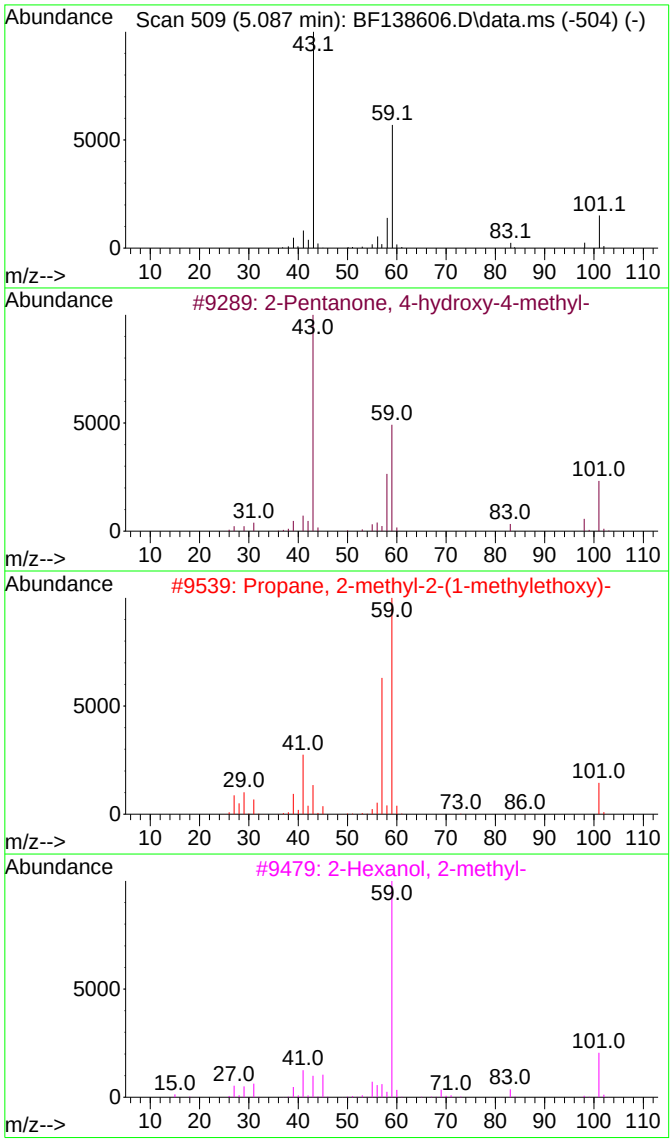
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

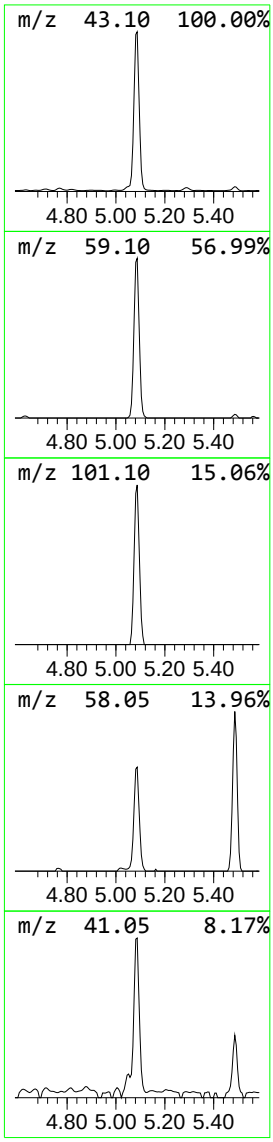
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	5.63 ng	196919	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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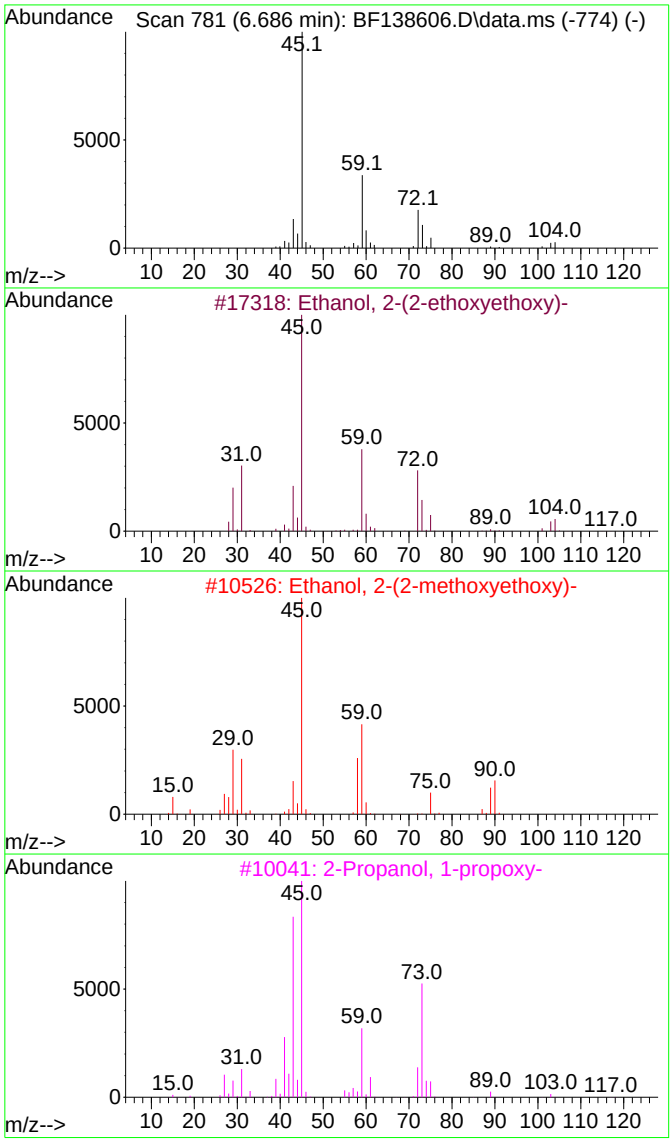
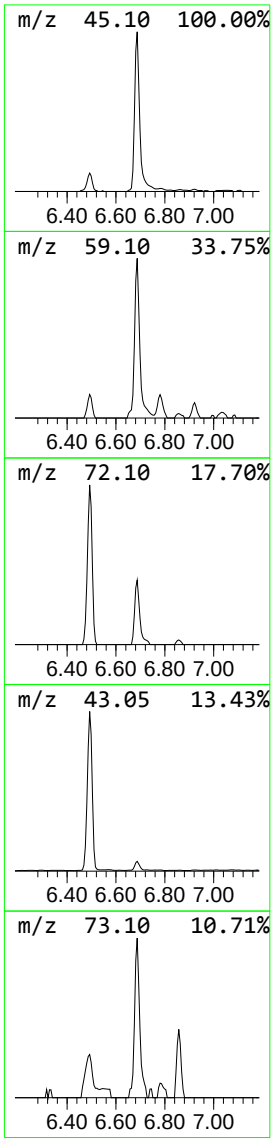
****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.686	2.77 ng	96795	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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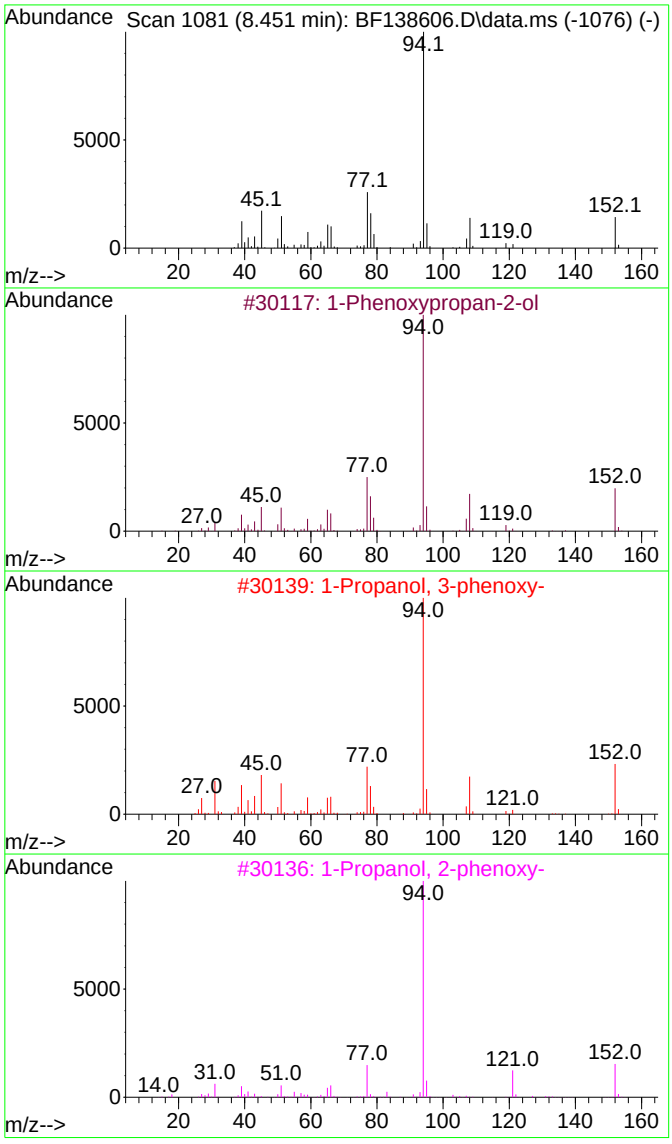
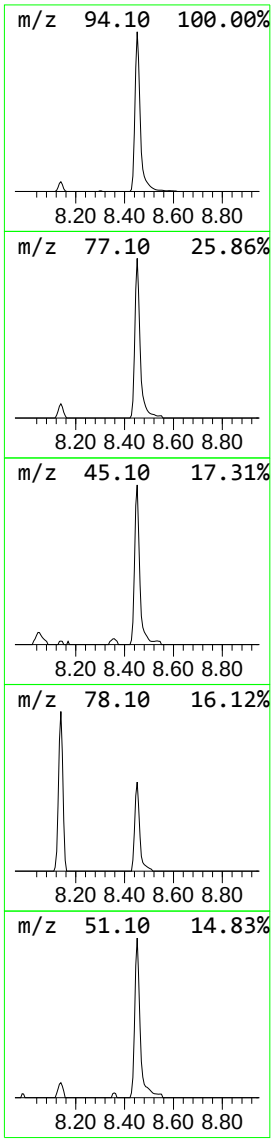
Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	5.45 ng	222647	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	59





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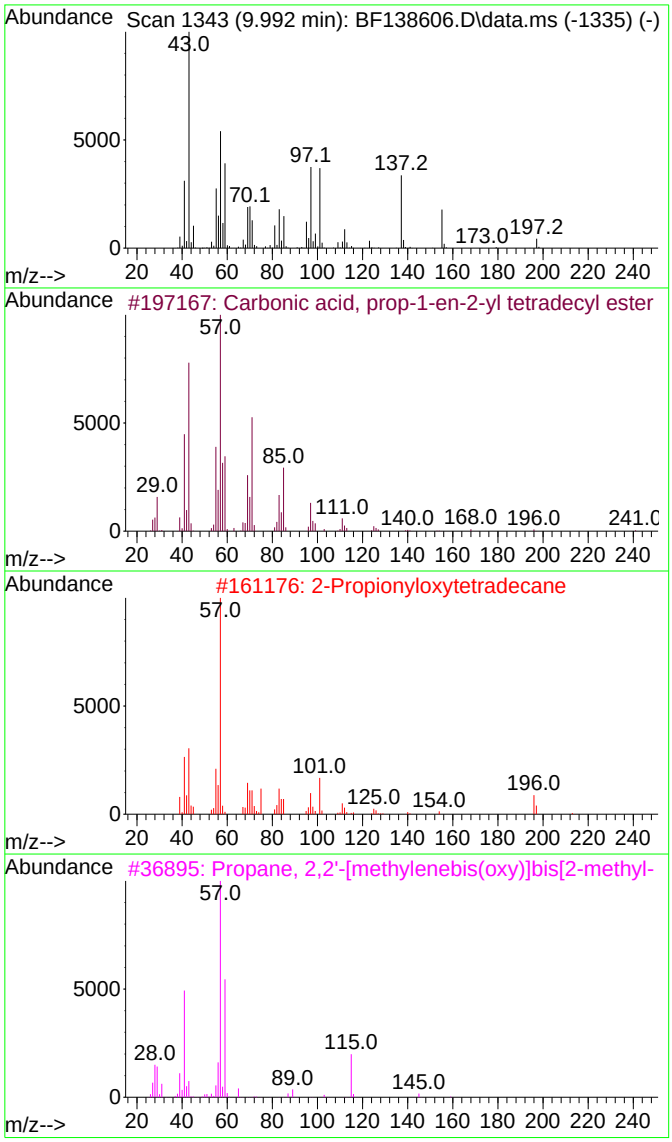
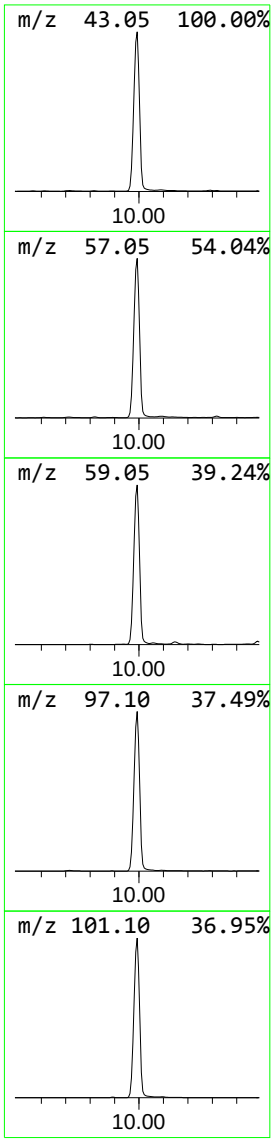
****

Peak Number 6 unknown9.992 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	52.79 ng	2524270	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	25
2	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	14
3	Propane, 2,2'-[methylenebis(oxy)...	160	C9H20O2	002568-93-6	10
4	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
5	11-Tricosene	322	C23H46	052078-56-5	10





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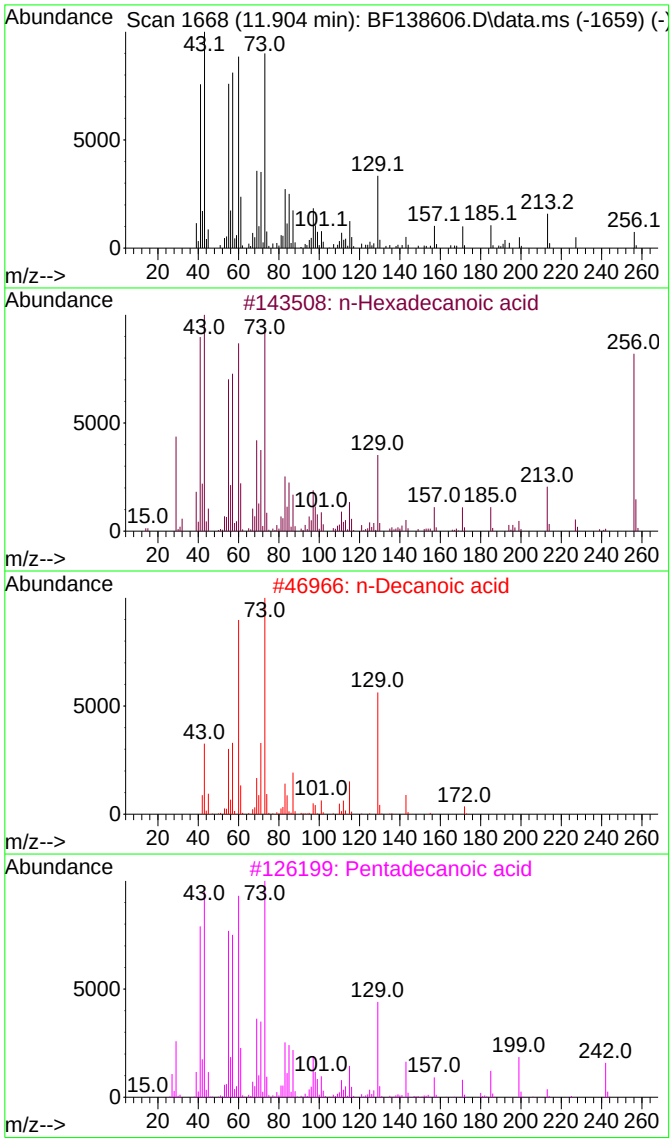
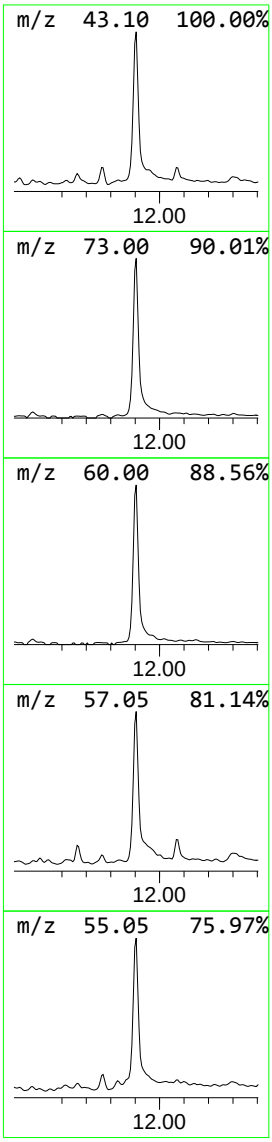
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	9.14 ng	346060	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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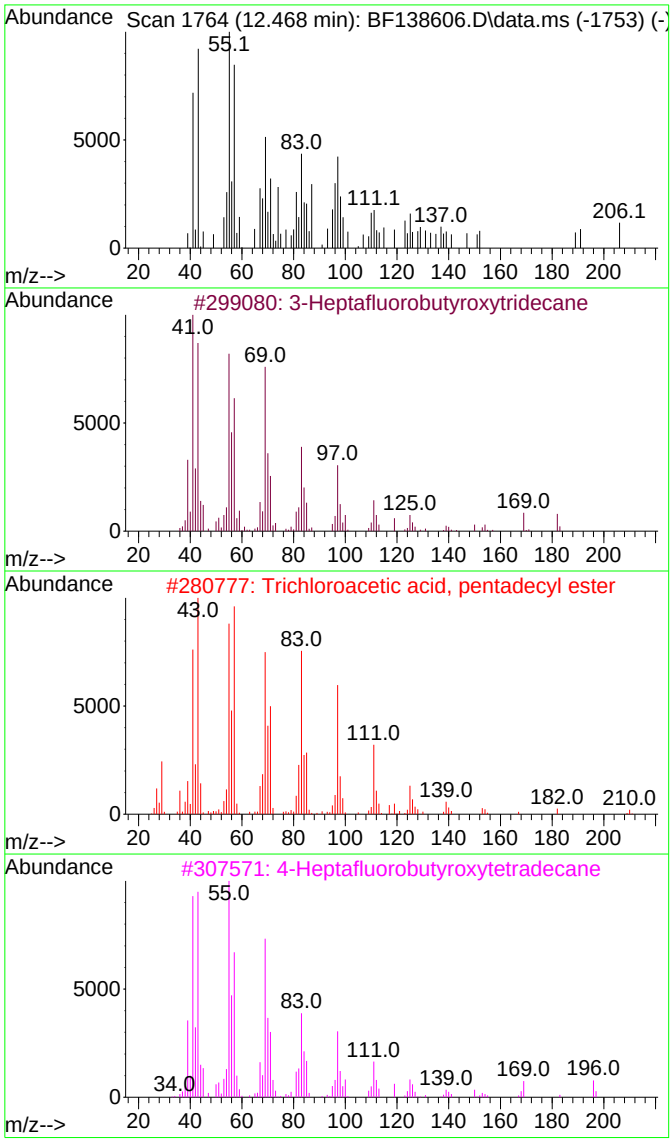
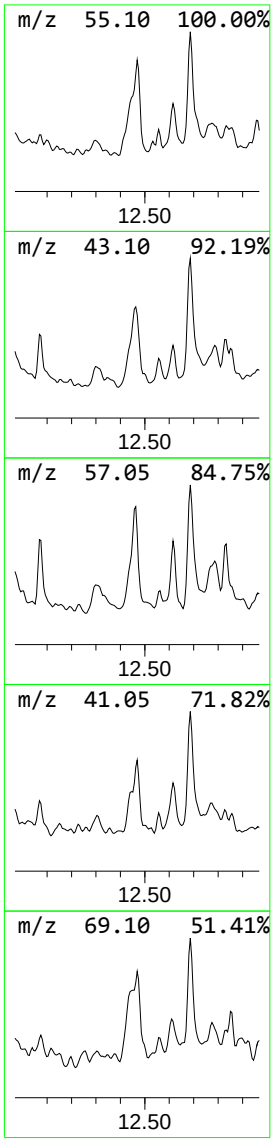
Peak Number 8 unknown12.469 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	2.17 ng	82133	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-5	49
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49
3	4-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-9	49
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	49
5	17-Pentatriacontene	491	C35H70	006971-40-0	49





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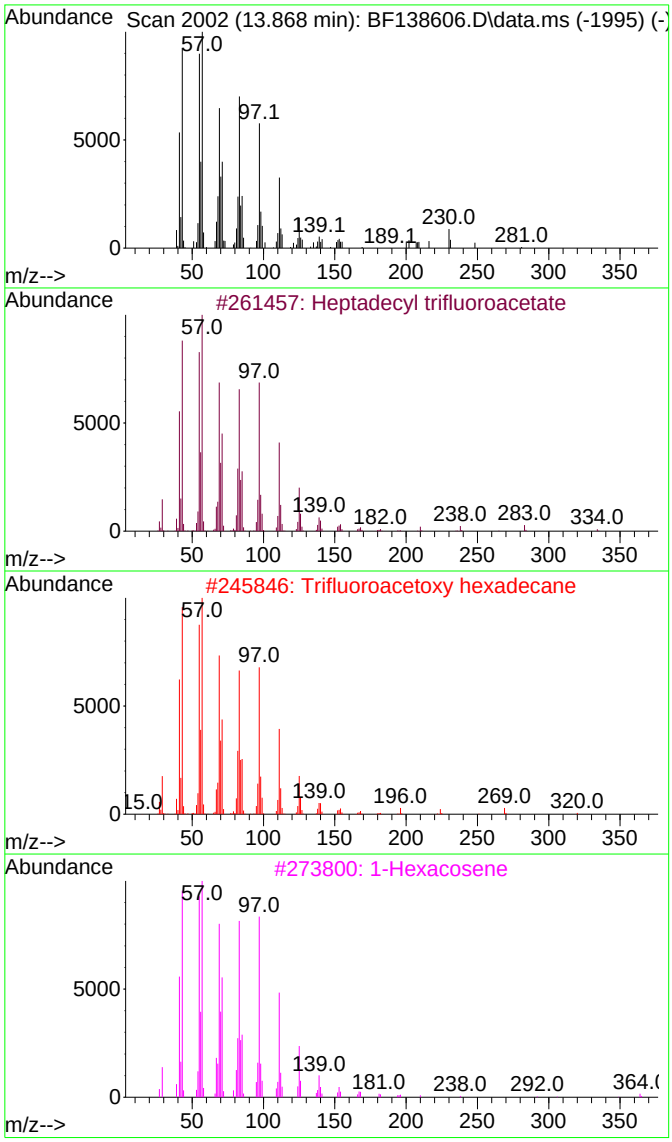
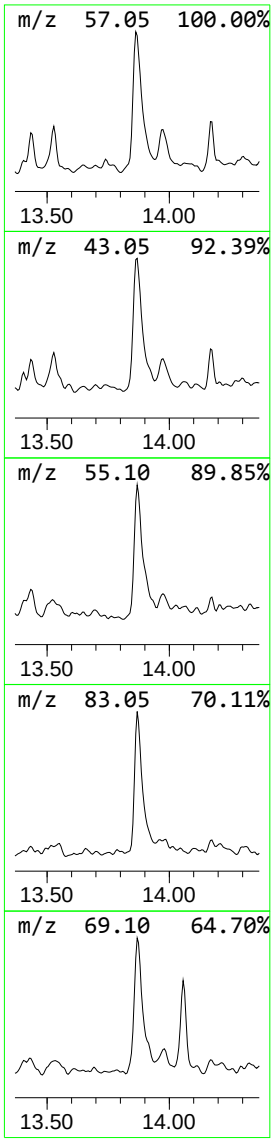
****
Peak Number 9 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	5.48 ng	155199	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





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Data File : BF138606.D
Acq On : 22 Jul 2024 14:14
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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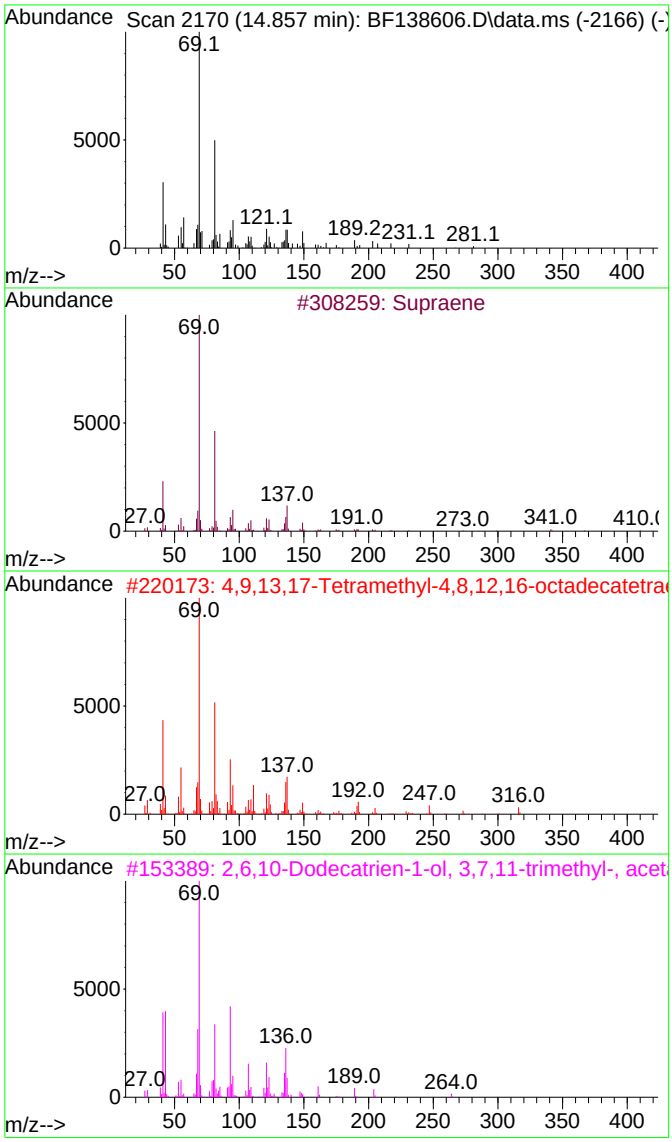
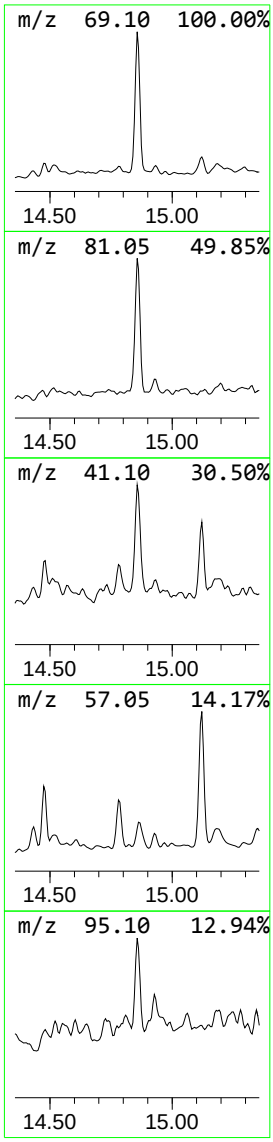
Peak Number 10 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	2.44 ng	61686	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072224\
Data File : BF138606.D
Acq On : 22 Jul 2024 14:14
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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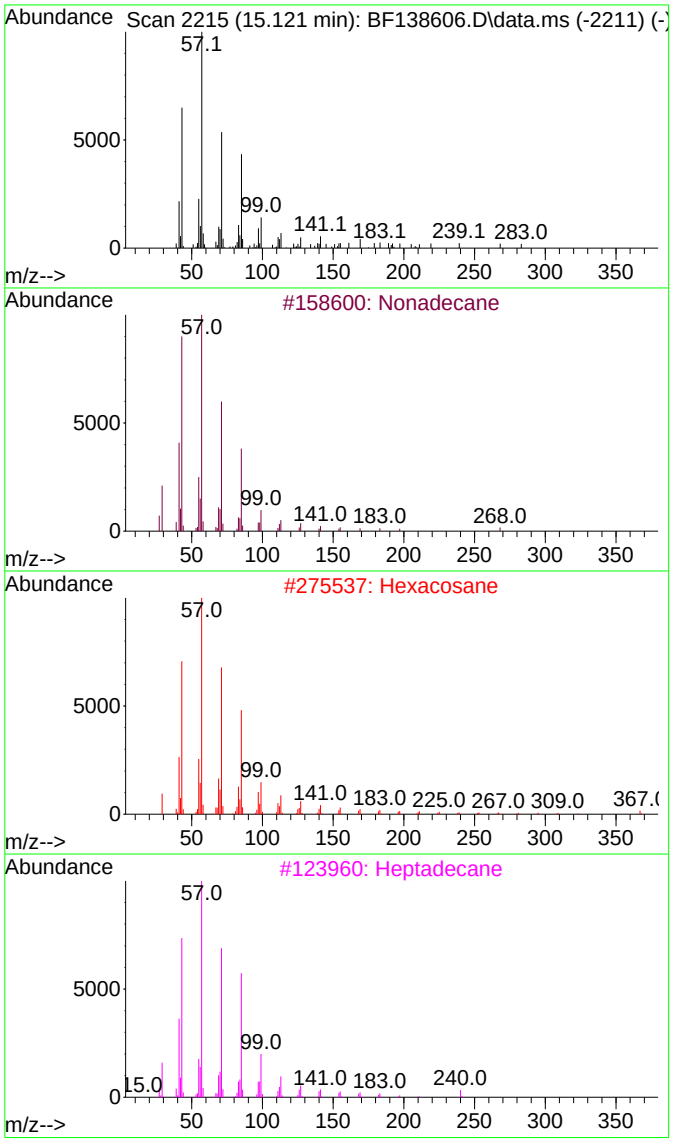
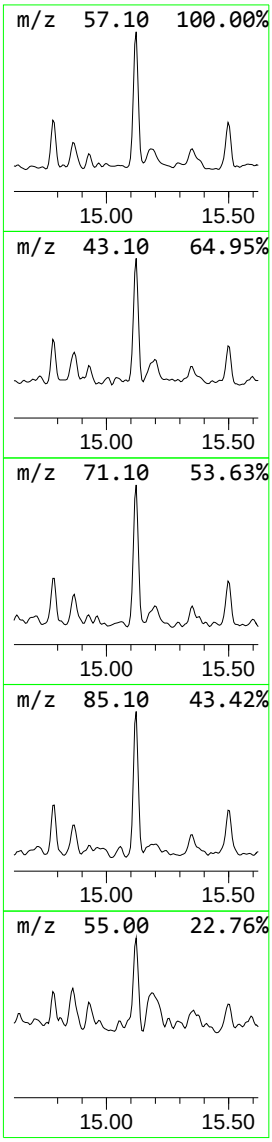
Peak Number 11 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	2.31 ng	58400	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072224\
Data File : BF138606.D
Acq On : 22 Jul 2024 14:14
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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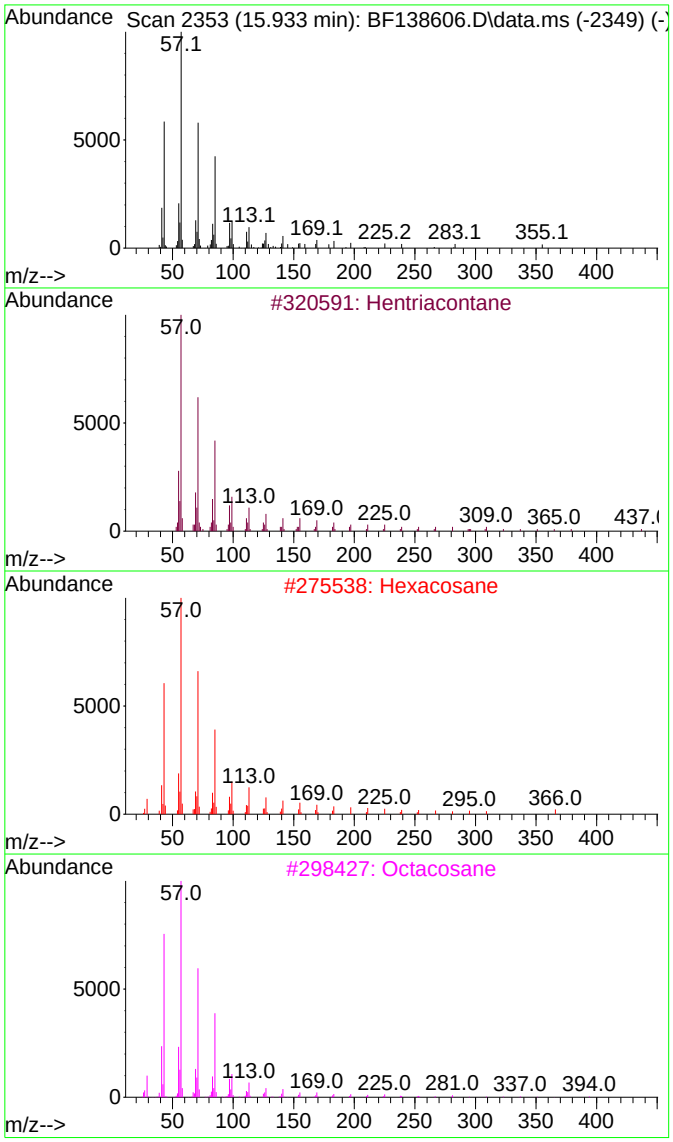
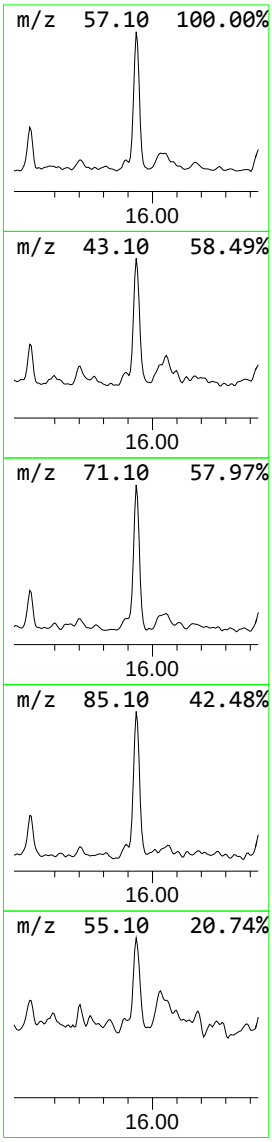
Peak Number 12 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	2.99 ng	75637	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Docosane	310	C22H46	000629-97-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072224\
Data File : BF138606.D
Acq On : 22 Jul 2024 14:14
Operator : RC/JU
Sample : P3302-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
285-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.175	67.3	ng	2350610	1	6.857	698915	20.0
Propylene Glycol	3.404	5.6	ng	196213	1	6.857	698915	20.0
2-Pentanone, 4-...	5.087	5.6	ng	196919	1	6.857	698915	20.0
Ethanol, 2-(2-e...	6.686	2.8	ng	96795	1	6.857	698915	20.0
1-Phenoxypropan...	8.451	5.5	ng	222647	2	8.139	817482	20.0
unknown9.992	9.992	52.8	ng	2524270	3	9.892	956405	20.0
n-Hexadecanoic ...	11.904	9.1	ng	346060	4	11.380	757230	20.0
unknown12.469	12.469	2.2	ng	82133	4	11.380	757230	20.0
Heptadecyl trif...	13.868	5.5	ng	155199	5	14.015	566496	20.0
Supraene	14.857	2.4	ng	61686	6	15.480	506067	20.0
Nonadecane	15.121	2.3	ng	58400	6	15.480	506067	20.0
Hentriacontane	15.933	3.0	ng	75637	6	15.480	506067	20.0