LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138745.D
Acq On : 02 Aug 2024 14:02
Operator : RC/JU
Sample : P3402-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-222

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	211	216	241	rBV	11432	44871	2.50%	0.384%
2	5.063	500	505	516	rVB	63252	93022	5.19%	0.797%
3	5.469	569	574	594	rBV	1037931	1355769	75.67%	11.617%
4	6.481	740	746	761	rBV	1194024	1575929	87.96%	13.503%
5	6.846	803	808	813	rVB	276554	346685	19.35%	2.970%
6	7.404	897	903	914	rBV	782089	1029208	57.44%	8.818%
7	7.657	941	946	955	rBV	21425	27100	1.51%	0.232%
8	8.122	1020	1025	1030	rBV	303935	373916	20.87%	3.204%
9	8.434	1074	1078	1094	rVB	46058	68221	3.81%	0.585%
10	9.198	1202	1208	1213	rBV	1462357	1791688	100.00%	15.352%
11	9.875	1318	1323	1328	rBV	396799	487591	27.21%	4.178%
12	9.969	1333	1339	1349	rBV	243172	363691	20.30%	3.116%
13	10.669	1452	1458	1471	rBV	660945	892374	49.81%	7.646%
14	11.363	1571	1576	1585	rBV	341680	435917	24.33%	3.735%
15	11.892	1658	1666	1678	rBV2	44004	87361	4.88%	0.749%
16	12.575	1778	1782	1793	rBV	22770	30271	1.69%	0.259%
17	12.675	1794	1799	1805	rBV3	11867	21178	1.18%	0.181%
18	12.804	1815	1821	1825	rBV2	20539	29733	1.66%	0.255%
19	12.945	1840	1845	1850	rBV	1046247	1315219	73.41%	11.269%
20	13.169	1879	1883	1887	rBV	11965	18403	1.03%	0.158%
21	13.510	1937	1941	1951	rVB2	11117	18031	1.01%	0.154%
22	13.851	1993	1999	2014	rBV2	50579	142255	7.94%	1.219%
23	13.974	2016	2020	2022	rVV	84725	118574	6.62%	1.016%
24	14.004	2022	2025	2038	rVB	227540	308903	17.24%	2.647%
25	14.463	2099	2103	2106	rBV	17619	27894	1.56%	0.239%
26	14.621	2127	2130	2135	rBV3	23917	41836	2.34%	0.358%
27	14.757	2149	2153	2158	rVB2	28783	57967	3.24%	0.497%
28	15.098	2207	2211	2216	rVB	21990	31978	1.78%	0.274%
29	15.163	2216	2222	2231	rBV9	15499	56051	3.13%	0.480%
30	15.463	2268	2273	2288	rBV	211850	338949	18.92%	2.904%
31	15.910	2343	2349	2356	rVB	33862	58539	3.27%	0.502%
32	16.021	2360	2368	2374	rBV9	12439	45956	2.56%	0.394%
33	16.998	2528	2534	2541	rVB3	15773	35958	2.01%	0.308%

Sum of corrected areas: 11671038

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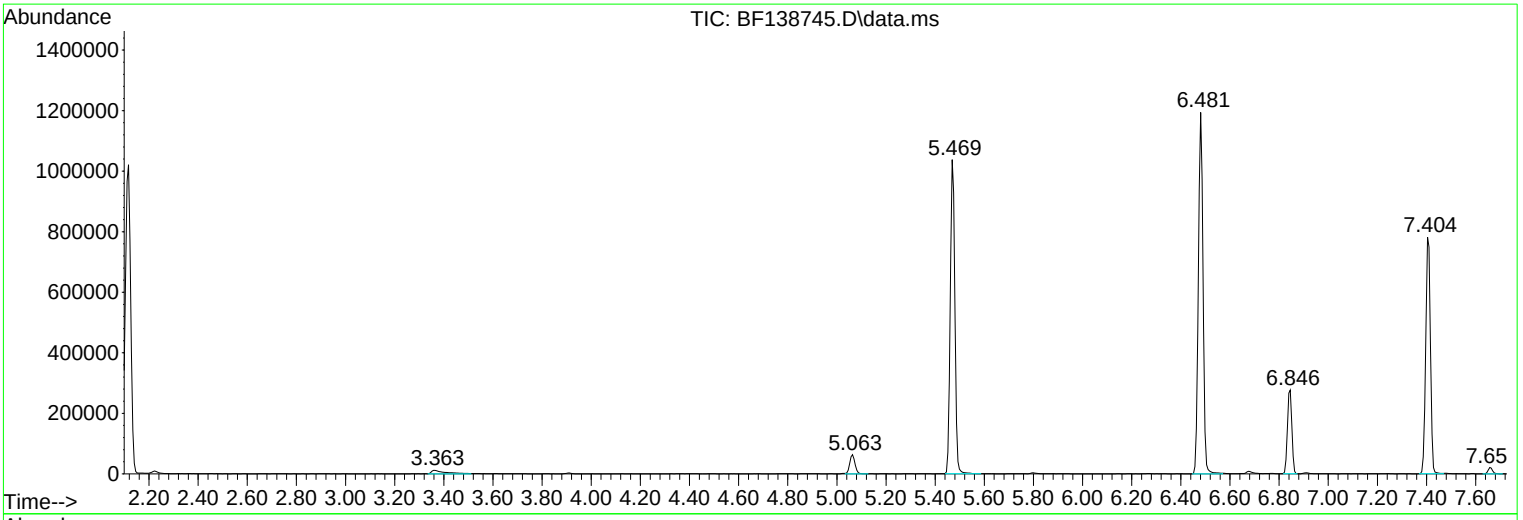
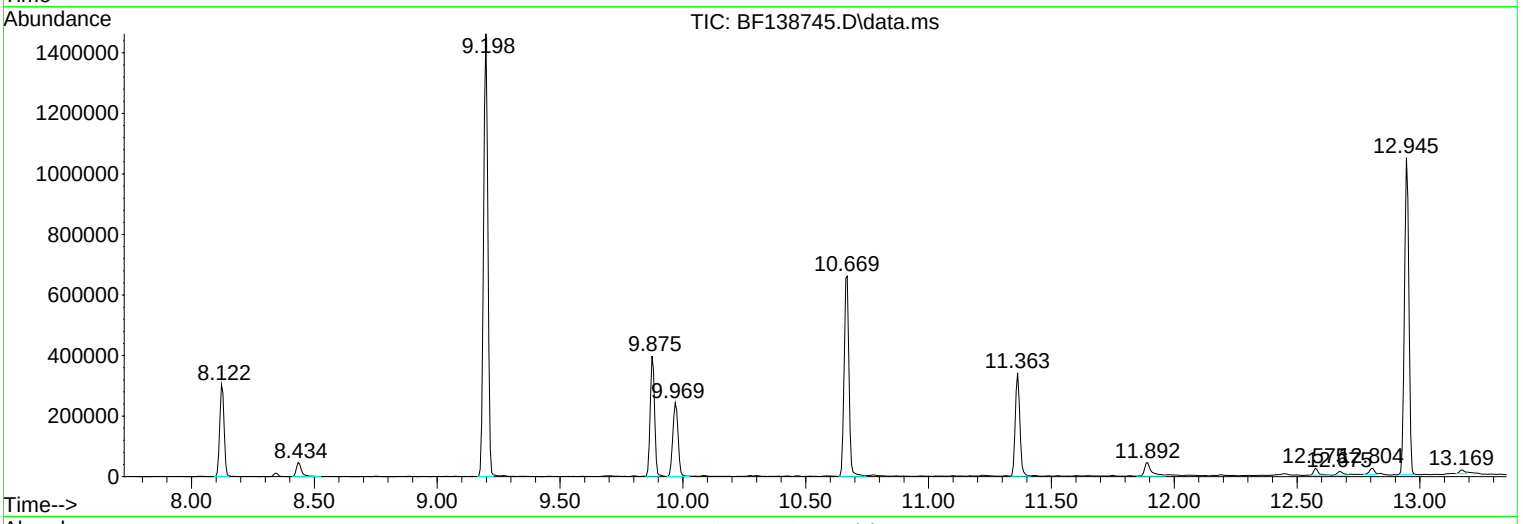
Misc :
ALS Vial : 11 Sample Multiplier: 1

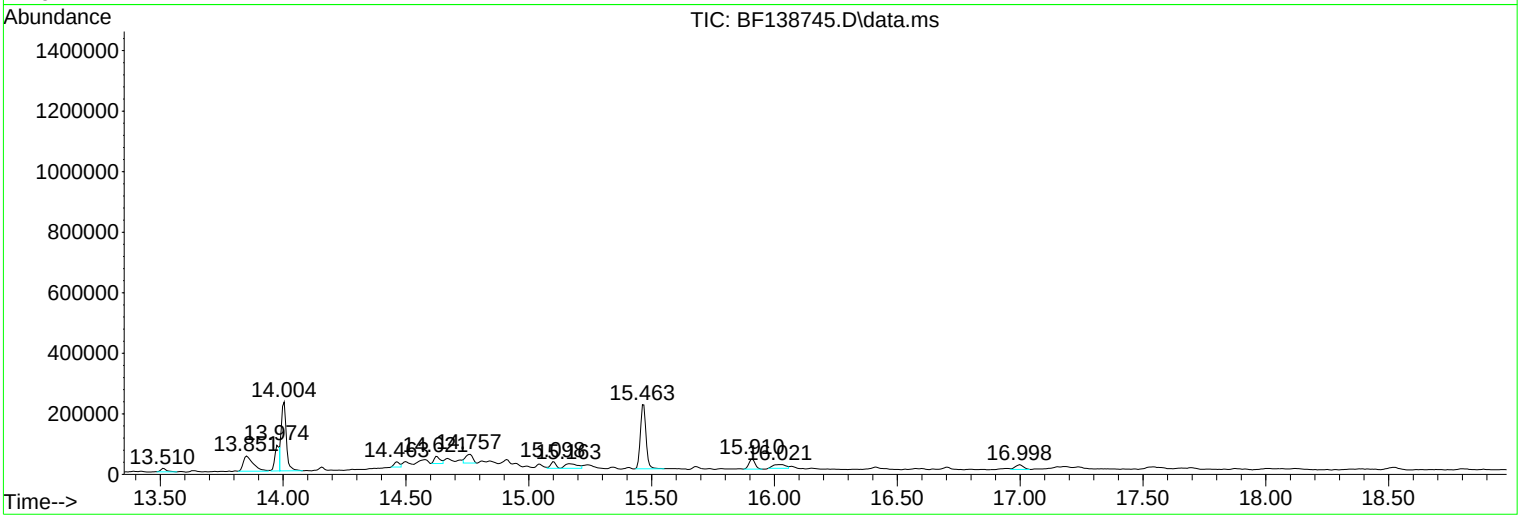
Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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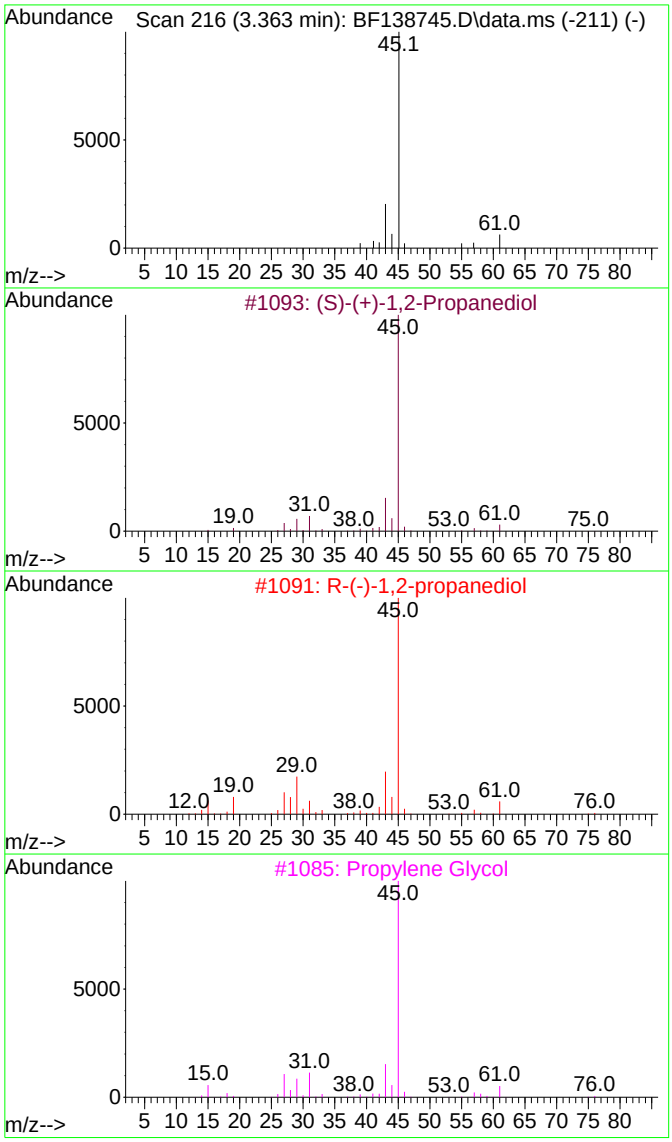
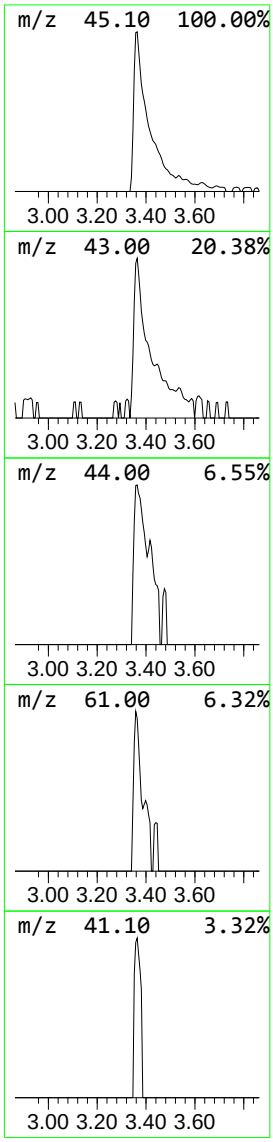
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	2.59 ng	44871	1,4-Dichlorobenzene-d4	6.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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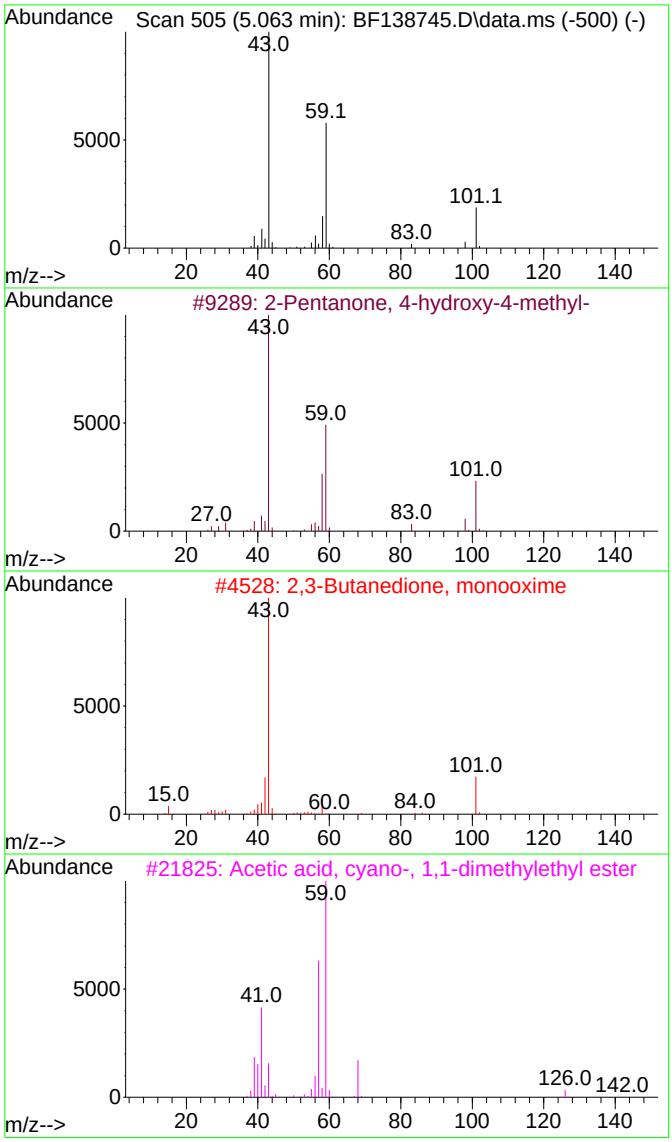
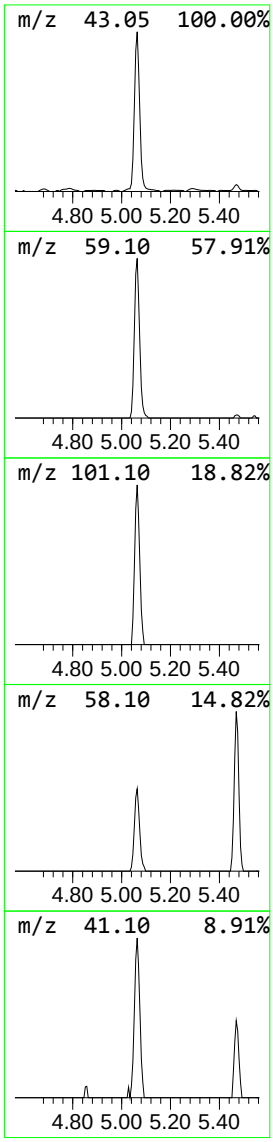
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.37 ng	93022	1,4-Dichlorobenzene-d4	6.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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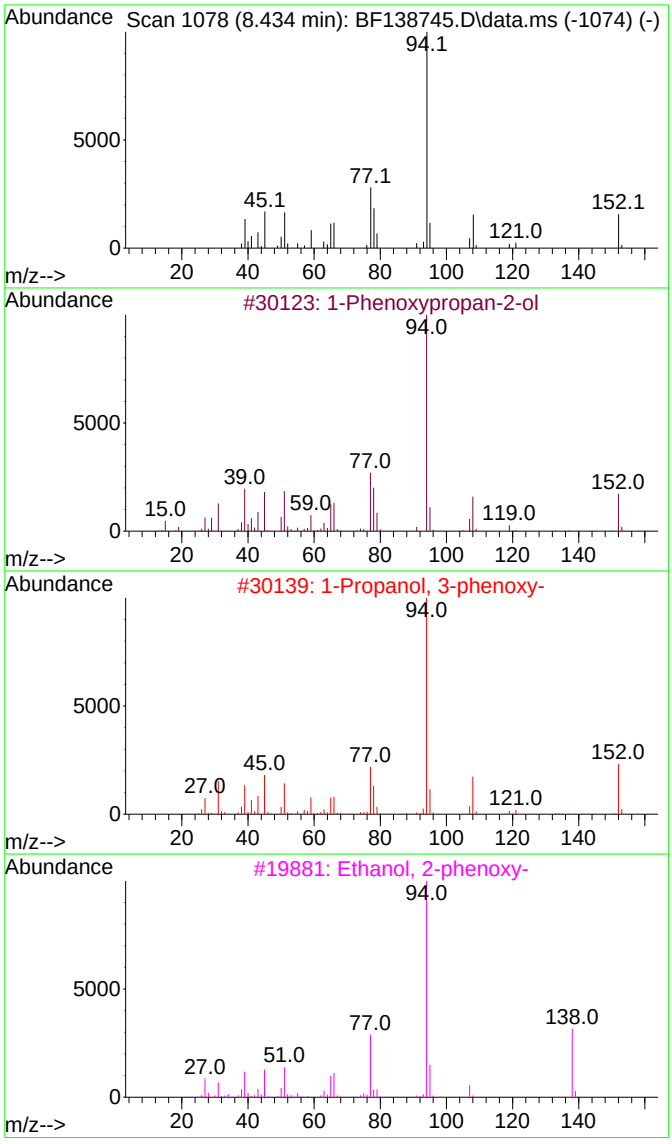
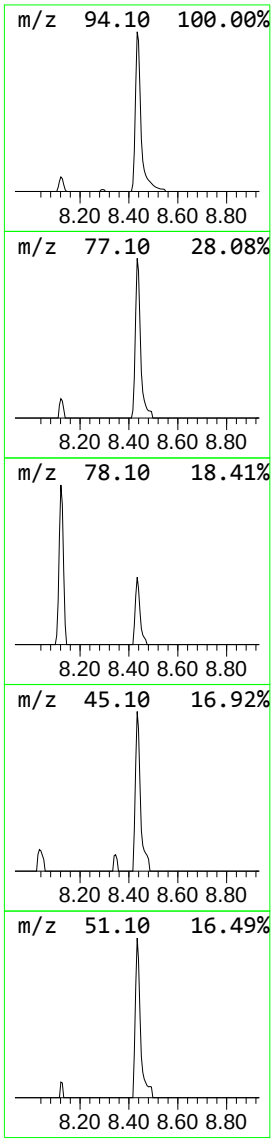
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	3.65 ng	68221	Naphthalene-d8	8.122

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	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





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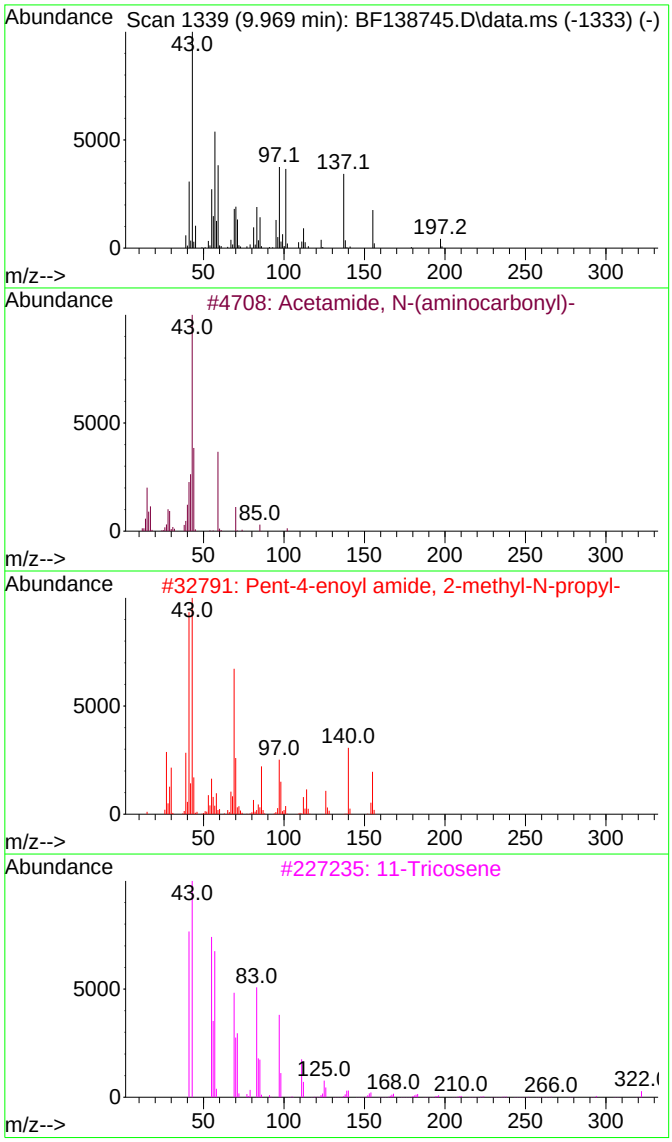
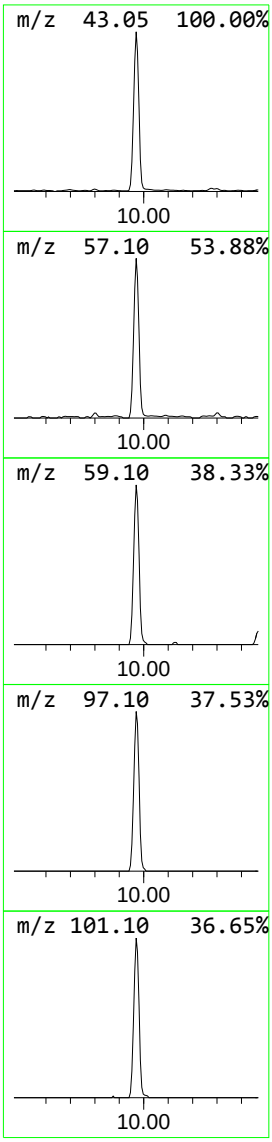
****

Peak Number 4 unknown9.969 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.969	14.92 ng	363691	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	16
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3	11-Tricosene	322	C23H46	052078-56-5	12
4	Dichloroacetic acid, nonyl ester	254	C11H20Cl2O2	083004-99-3	10
5	Diethylmalonic acid, monochlorid...	318	C17H31ClO3	1000369-41-8	10





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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TIC Library : C:\Database\NIST20.L
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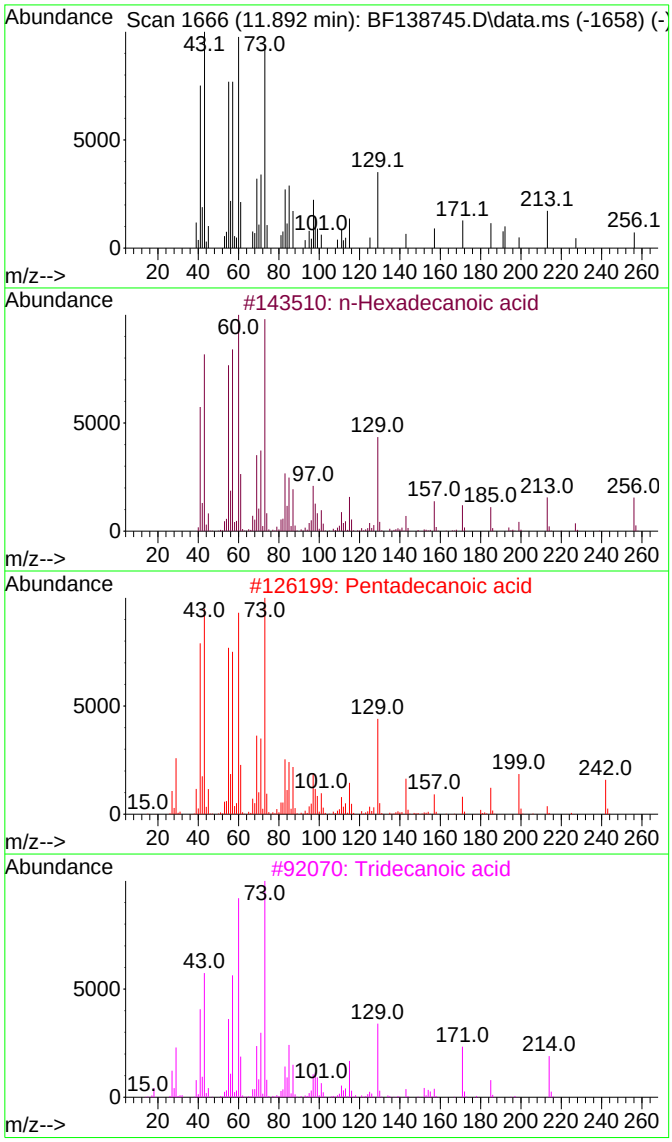
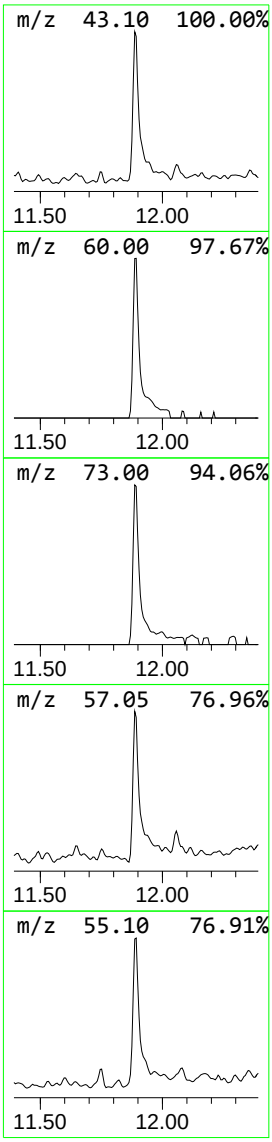
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.01 ng	87361	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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TIC Library : C:\Database\NIST20.L
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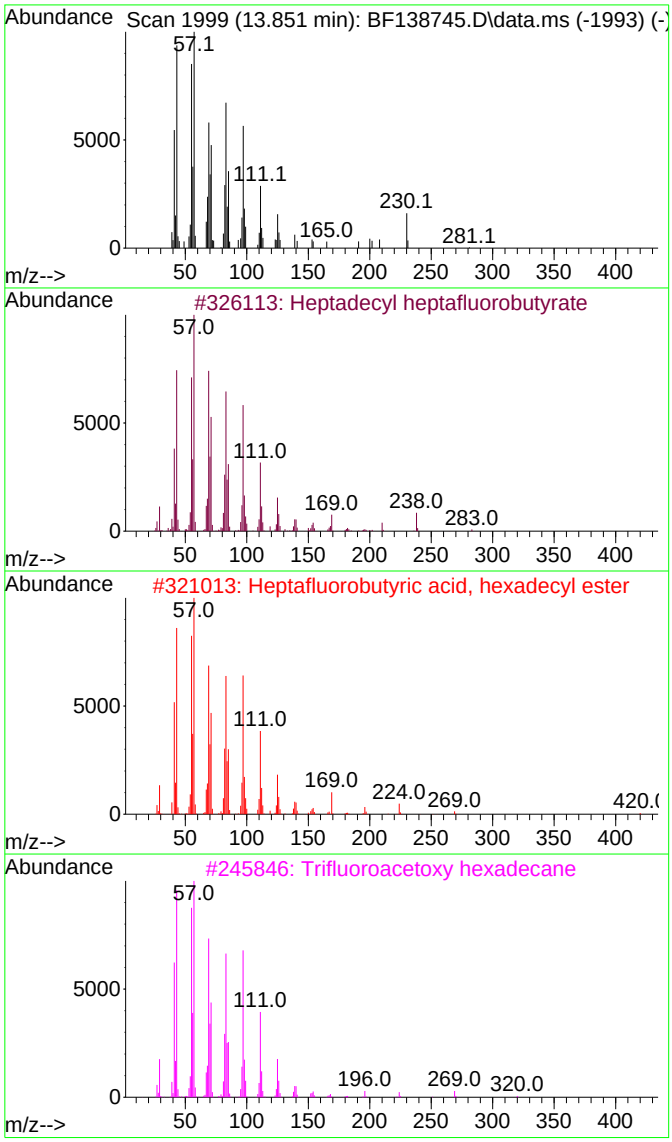
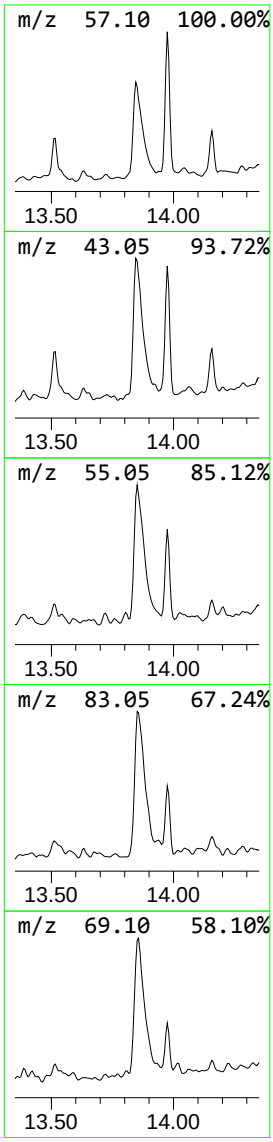
****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	9.21 ng	142255	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	1-Hexacosanol	382	C26H54O	000506-52-5	90
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90





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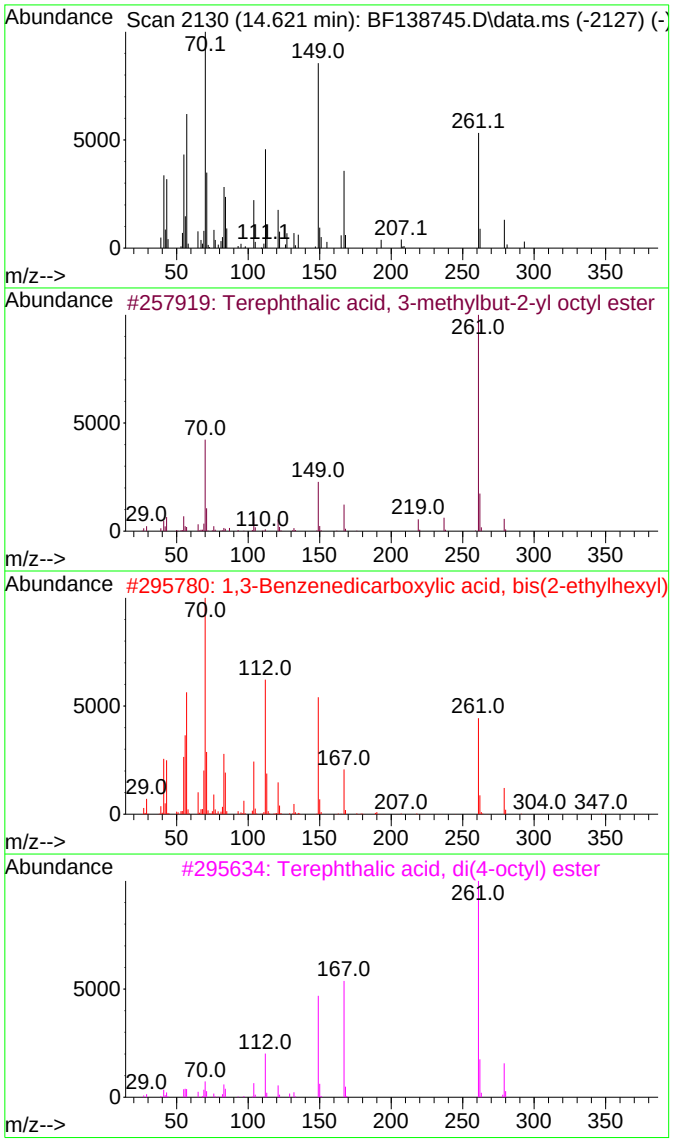
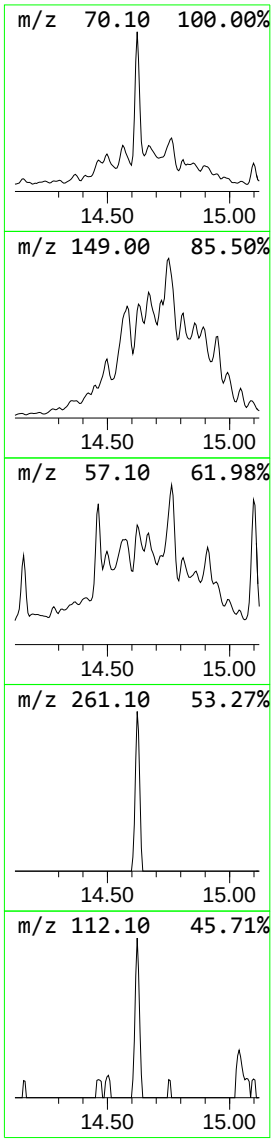
****
Peak Number 7 Terephthalic acid, 3-methyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	2.71 ng	41836	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	47
4	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	43
5	Isophthalic acid, octyl undec-2-...	430	C27H42O4	1000343-91-0	38





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TIC Library : C:\Database\NIST20.L
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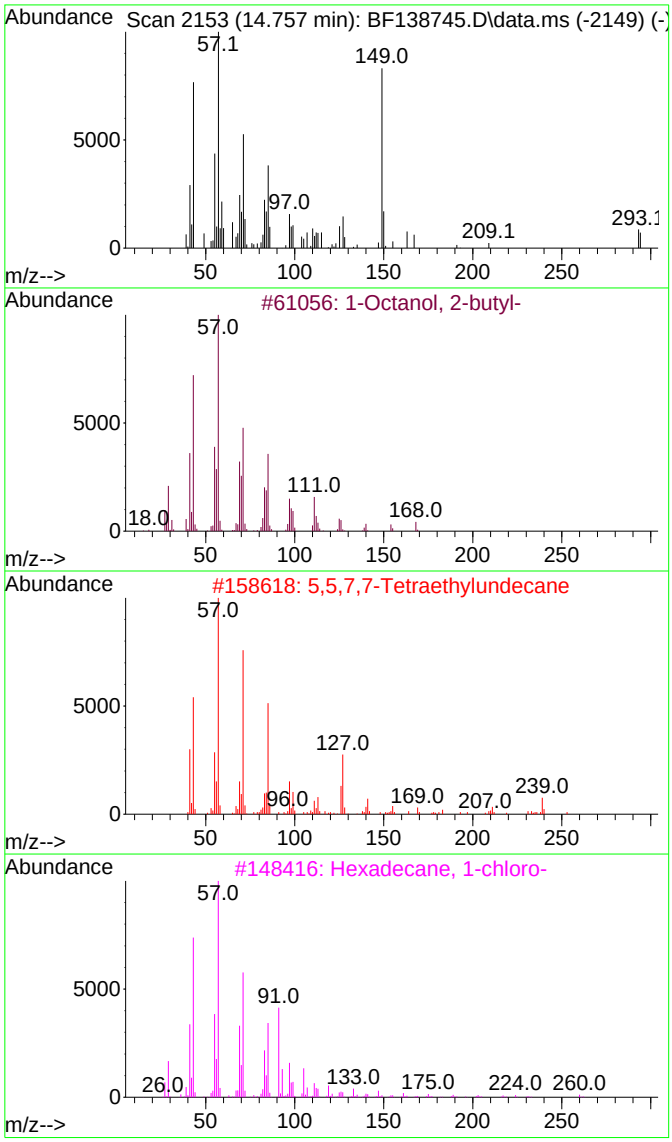
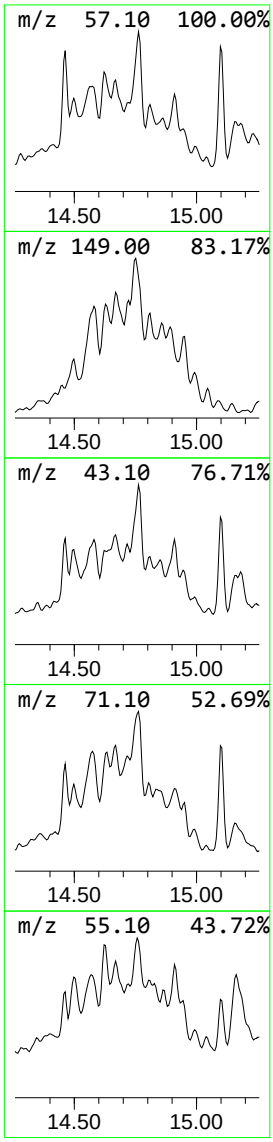
Peak Number 8 unknown14.757 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	3.42 ng	57967	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	30
2	5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	27
3	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	25
4	Docosane	310	C22H46	000629-97-0	22
5	Pentacosane	352	C25H52	000629-99-2	22





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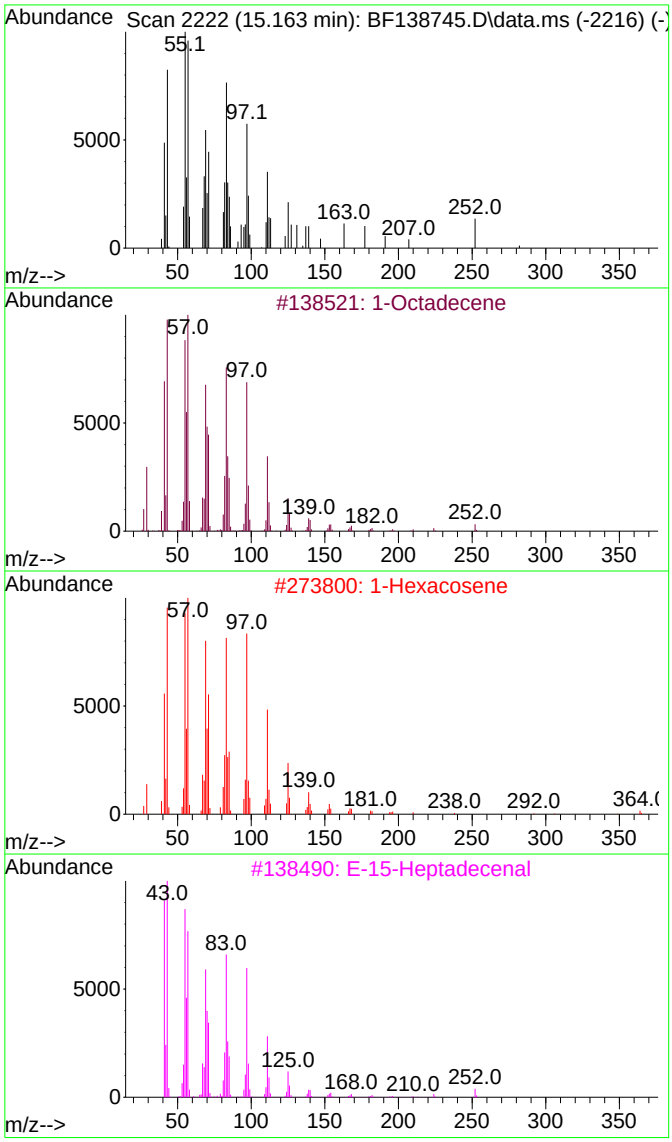
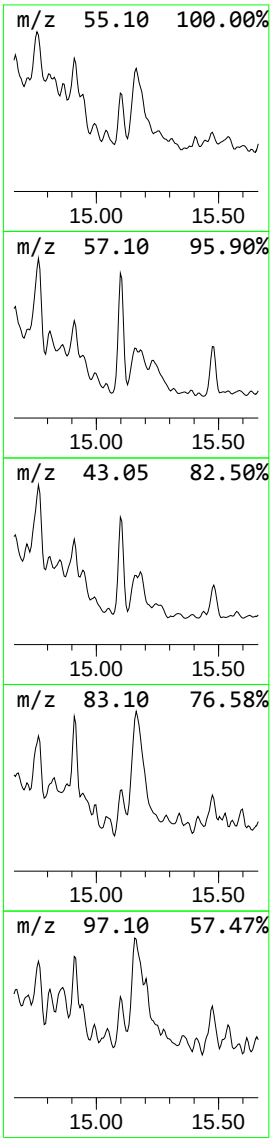
Peak Number 9 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	3.31 ng	56051	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	1-Hexacosene	364	C26H52	018835-33-1	87
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	74
4	1-Hexadecanol	242	C16H34O	036653-82-4	74
5	1-Heneicosanol	312	C21H44O	015594-90-8	64





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Data File : BF138745.D
Acq On : 02 Aug 2024 14:02
Operator : RC/JU
Sample : P3402-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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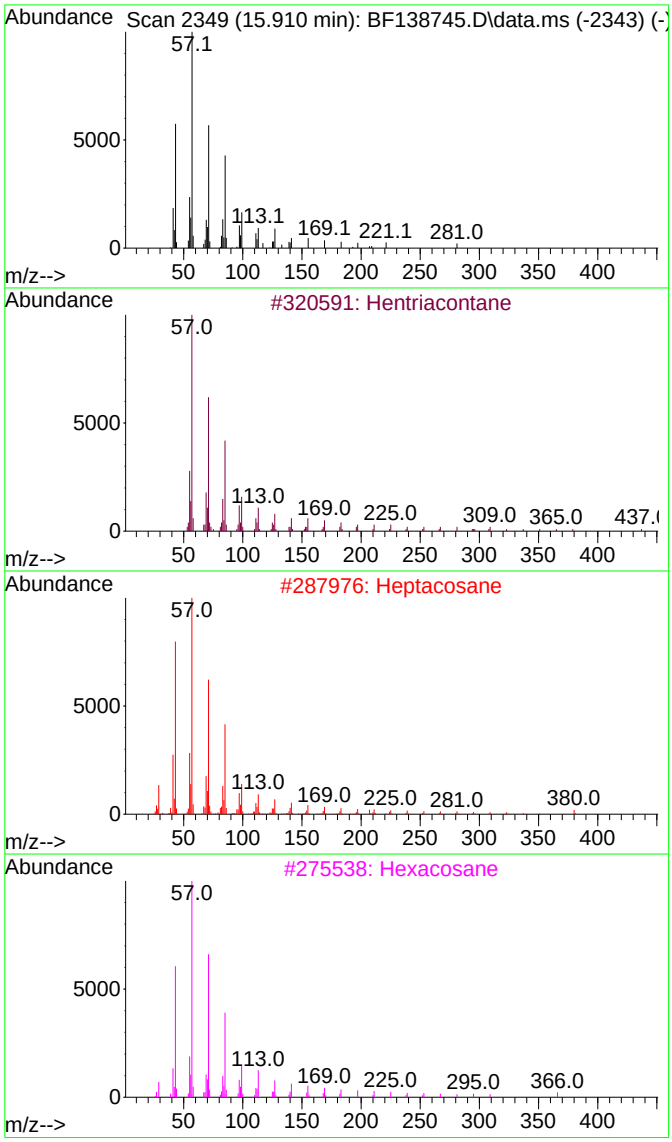
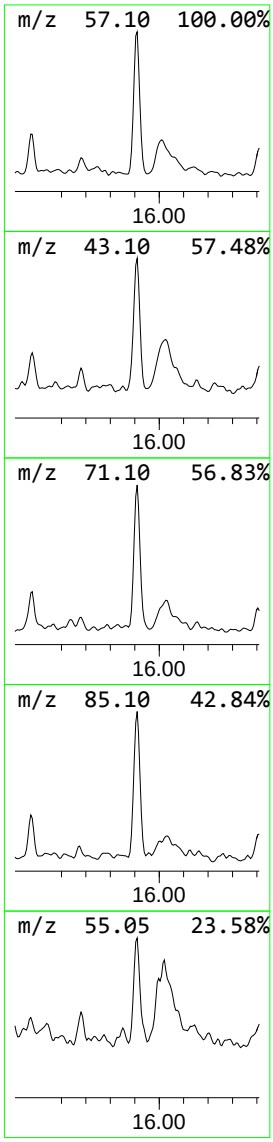
Peak Number 10 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	3.45 ng	58539	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	95
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Data File : BF138745.D
Acq On : 02 Aug 2024 14:02
Operator : RC/JU
Sample : P3402-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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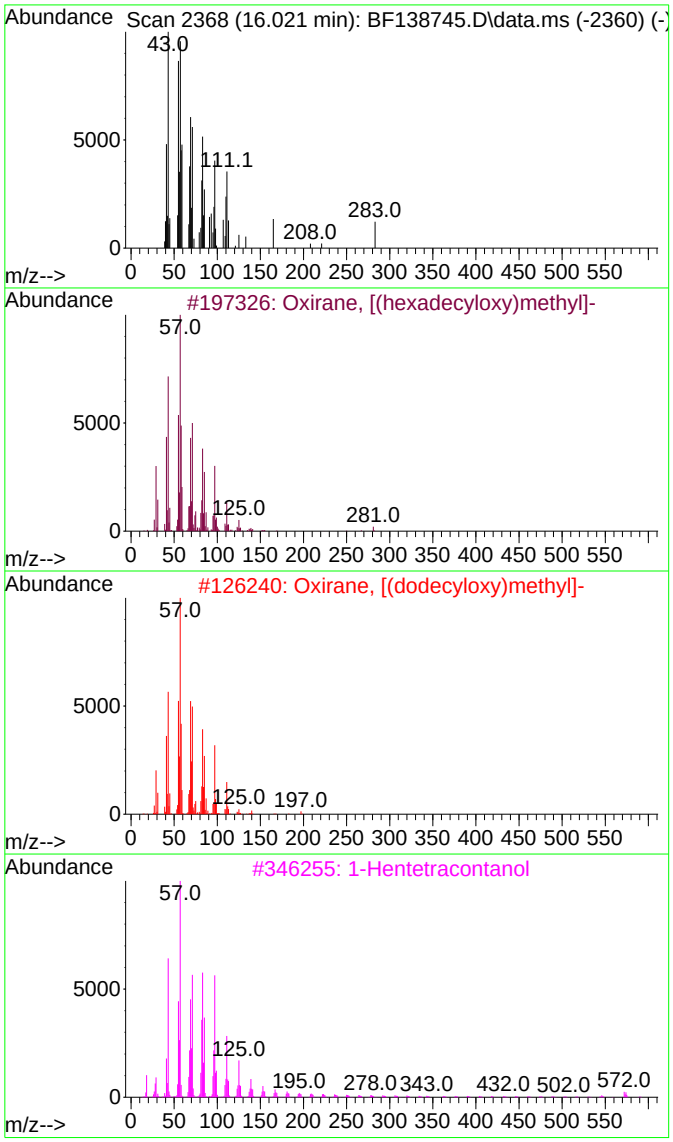
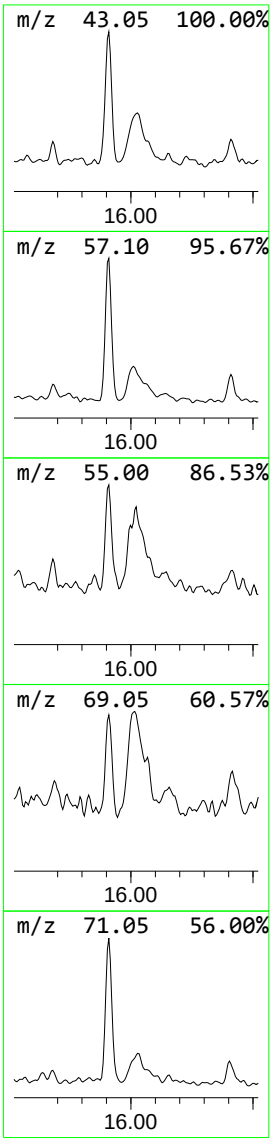
Peak Number 11 Oxirane, [(hexadecyloxy)met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	2.71 ng	45956	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	58
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	58
3	1-Hentetracontanol	593	C41H84O	040710-42-7	49
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	47
5	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138745.D
Acq On : 02 Aug 2024 14:02
Operator : RC/JU
Sample : P3402-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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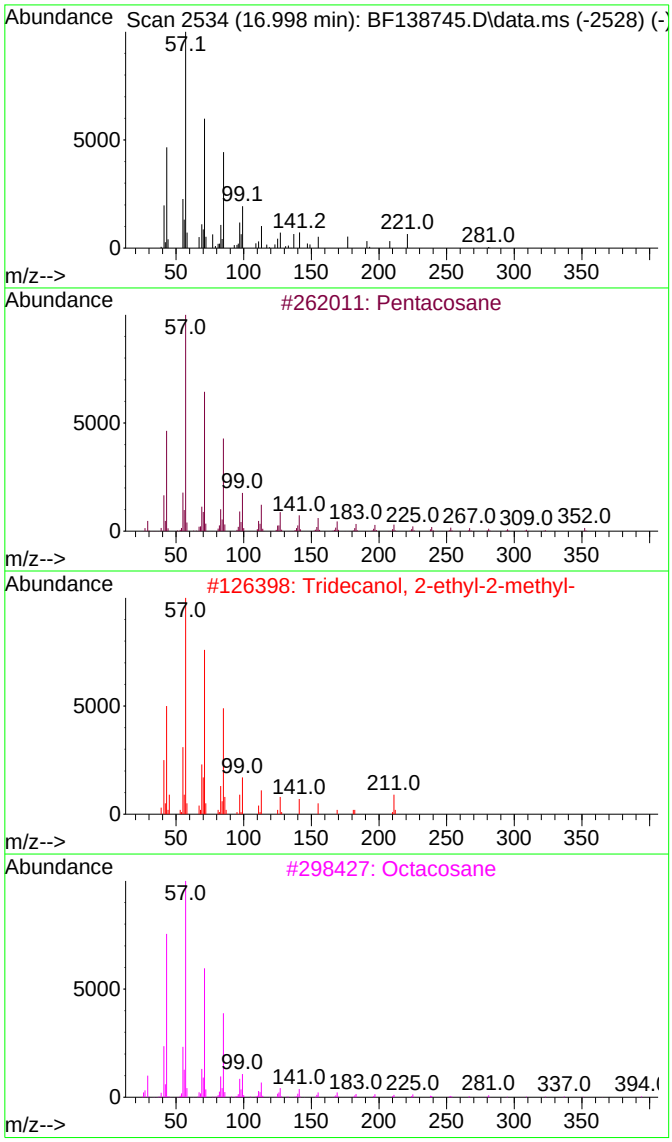
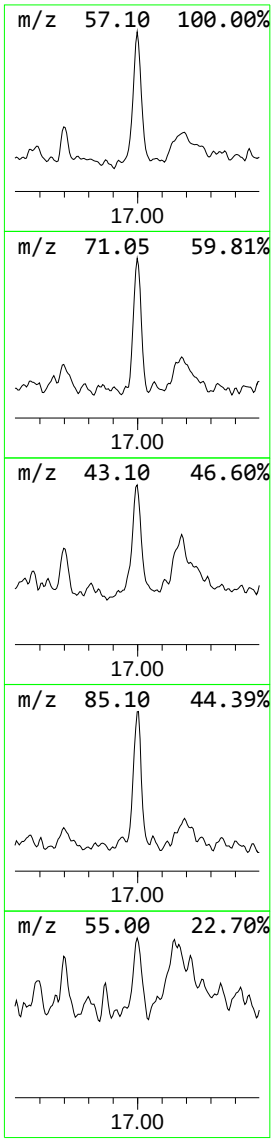
Peak Number 12 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.998	2.12 ng	35958	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	86
3	Octacosane	394	C28H58	000630-02-4	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138745.D
Acq On : 02 Aug 2024 14:02
Operator : RC/JU
Sample : P3402-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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
(S)-(+)-1,2-Pro...	3.363	2.6	ng	44871	1	6.846	346685	20.0
2-Pentanone, 4-...	5.063	5.4	ng	93022	1	6.846	346685	20.0
1-Phenoxypropan...	8.434	3.6	ng	68221	2	8.122	373916	20.0
unknown9.969	9.969	14.9	ng	363691	3	9.875	487591	20.0
n-Hexadecanoic ...	11.892	4.0	ng	87361	4	11.363	435917	20.0
Heptadecyl hept...	13.851	9.2	ng	142255	5	14.004	308903	20.0
Terephthalic ac...	14.621	2.7	ng	41836	5	14.004	308903	20.0
unknown14.757	14.757	3.4	ng	57967	6	15.463	338949	20.0
1-Octadecene	15.163	3.3	ng	56051	6	15.463	338949	20.0
Hentriacontane	15.910	3.5	ng	58539	6	15.463	338949	20.0
Oxirane, [(hexa...	16.021	2.7	ng	45956	6	15.463	338949	20.0
Pentacosane	16.998	2.1	ng	35958	6	15.463	338949	20.0