LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125864.D
Acq On : 15 Oct 2021 15:54
Operator : JU/CG
Sample : M4240-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-03-101421

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	15	rVB	1452824	2021545	37.85%	5.456%
2	5.069	504	507	514	rVB	62423	82693	1.55%	0.223%
3	5.457	568	573	576	rBV	3867146	4260556	79.78%	11.500%
4	6.463	738	744	747	rBV	3652378	4324916	80.98%	11.673%
5	6.833	803	807	810	rBV	1309279	989845	18.53%	2.672%
6	7.392	897	902	905	rBV	2659670	2867125	53.69%	7.739%
7	8.016	1004	1008	1020	rBV	727080	623750	11.68%	1.684%
8	8.110	1020	1024	1028	rBV	1405271	1338580	25.06%	3.613%
9	9.192	1202	1208	1211	rBV	5104488	5340475	100.00%	14.414%
10	9.527	1261	1265	1267	rBV	79229	65420	1.22%	0.177%
11	9.863	1315	1322	1326	rBV	1586772	1405851	26.32%	3.795%
12	10.651	1451	1456	1459	rBV	2970255	2693041	50.43%	7.269%
13	11.345	1570	1574	1577	rBV	1373151	1180352	22.10%	3.186%
14	11.368	1577	1578	1581	rVV	135728	81105	1.52%	0.219%
15	11.874	1661	1664	1670	rVB	287883	255367	4.78%	0.689%
16	12.557	1777	1780	1783	rBV	199649	167256	3.13%	0.451%
17	12.657	1794	1797	1803	rBV2	154084	176834	3.31%	0.477%
18	12.786	1815	1819	1821	rVB	146761	147375	2.76%	0.398%
19	12.933	1839	1844	1847	rBV	4636104	4328337	81.05%	11.683%
20	13.686	1969	1972	1976	rBV	160370	148732	2.78%	0.401%
21	13.833	1992	1997	1999	rBV3	269892	383511	7.18%	1.035%
22	13.980	2017	2022	2025	rBV	1298089	1205166	22.57%	3.253%
23	14.468	2100	2105	2115	rBV5	177035	394898	7.39%	1.066%
24	14.898	2175	2178	2184	rVB	121958	121664	2.28%	0.328%
25	15.009	2194	2197	2205	rBV	94837	179526	3.36%	0.485%
26	15.092	2208	2211	2213	rBV	127341	125299	2.35%	0.338%
27	15.121	2213	2216	2223	rVV2	205293	315462	5.91%	0.851%
28	15.303	2245	2247	2254	rVB	74215	95089	1.78%	0.257%
29	15.368	2255	2258	2261	rVV	77721	81734	1.53%	0.221%
30	15.433	2265	2269	2273	rVV	895382	1101189	20.62%	2.972%
31	15.462	2273	2274	2280	rVB2	107777	116022	2.17%	0.313%
32	15.668	2306	2309	2312	rVB5	52656	64759	1.21%	0.175%
33	15.898	2344	2348	2353	rBV	149544	208464	3.90%	0.563%
34	15.962	2355	2359	2367	rVV7	71568	157749	2.95%	0.426%

Sum of corrected areas: 37049687

Instrument :
BNA_F
ClientSampleId :
OR-03-101421

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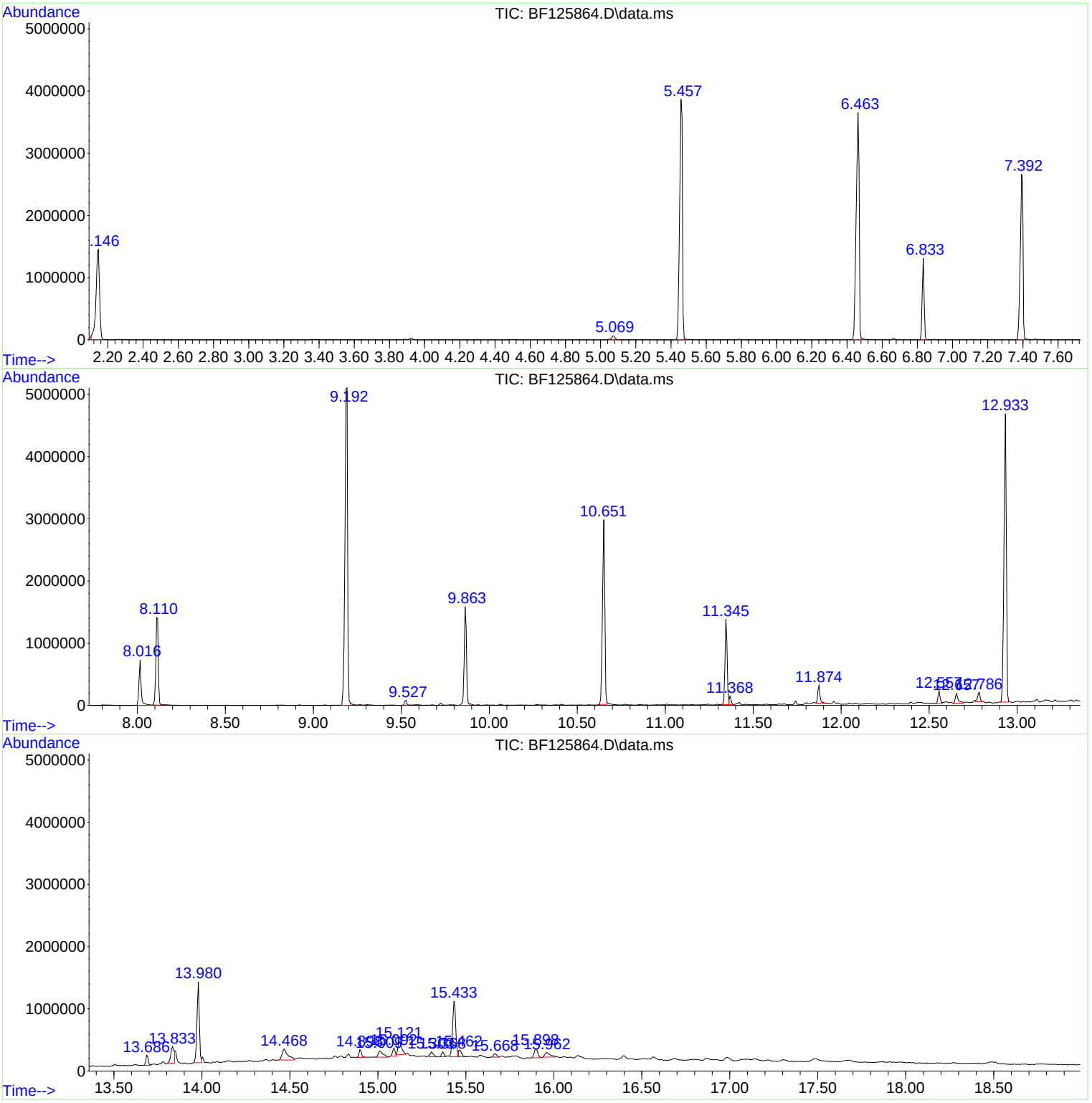
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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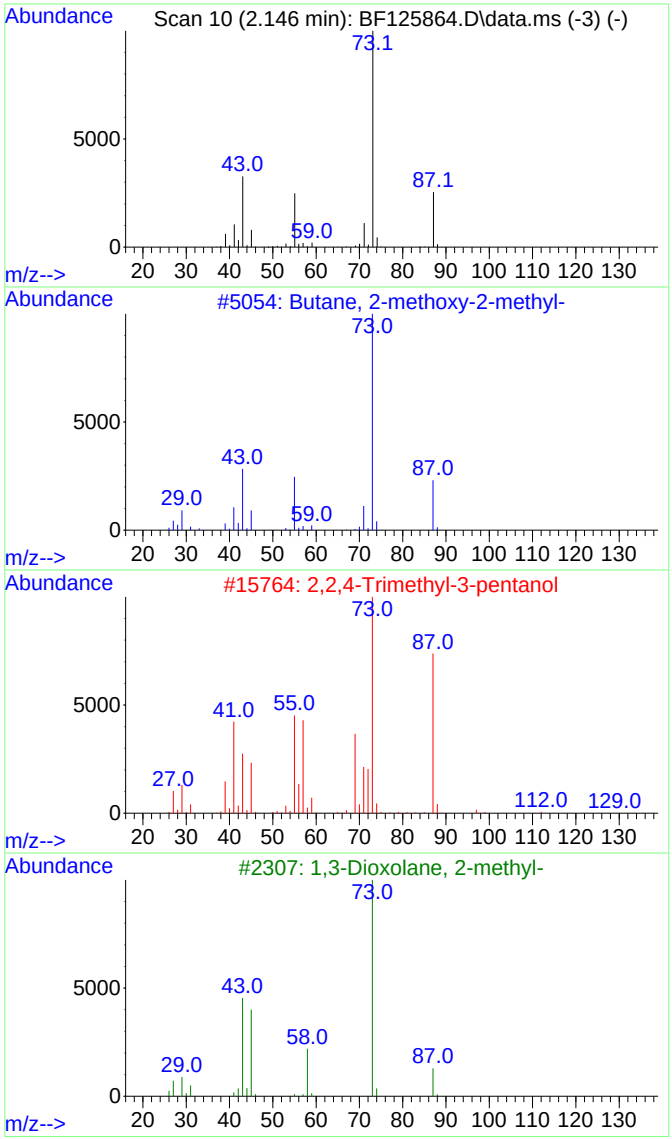
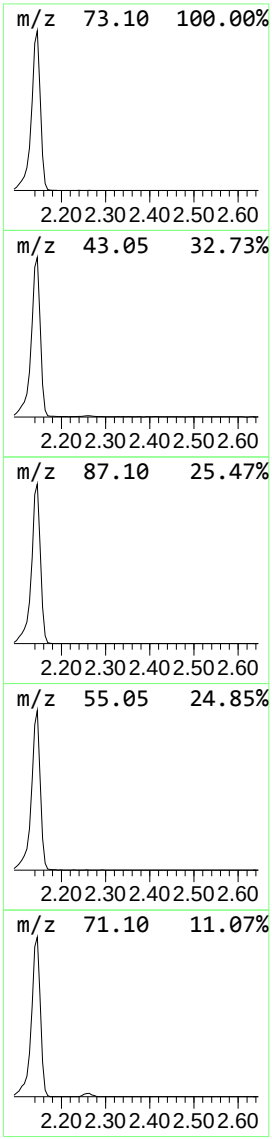
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	40.85 ng	2021550	1,4-Dichlorobenzene-d4	6.833

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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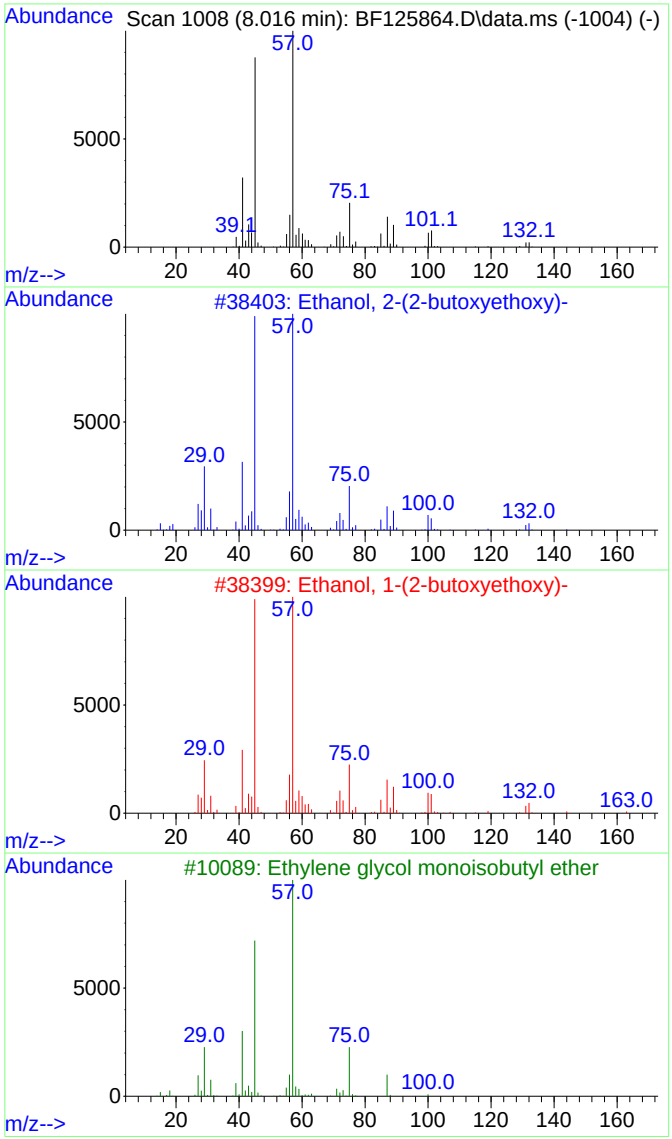
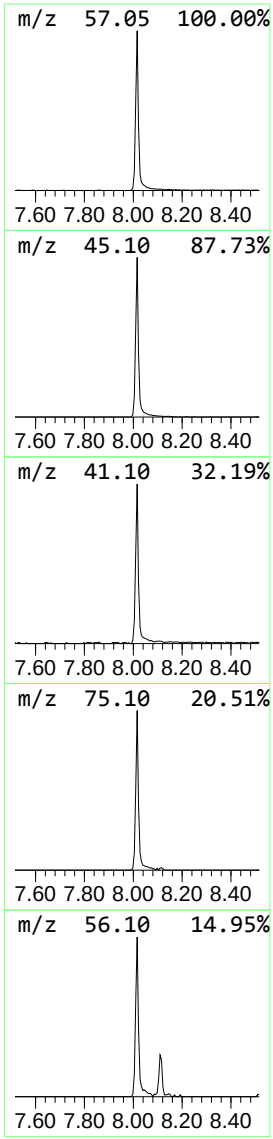
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	9.32 ng	623750	Naphthalene-d8	8.116

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	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-03-101421

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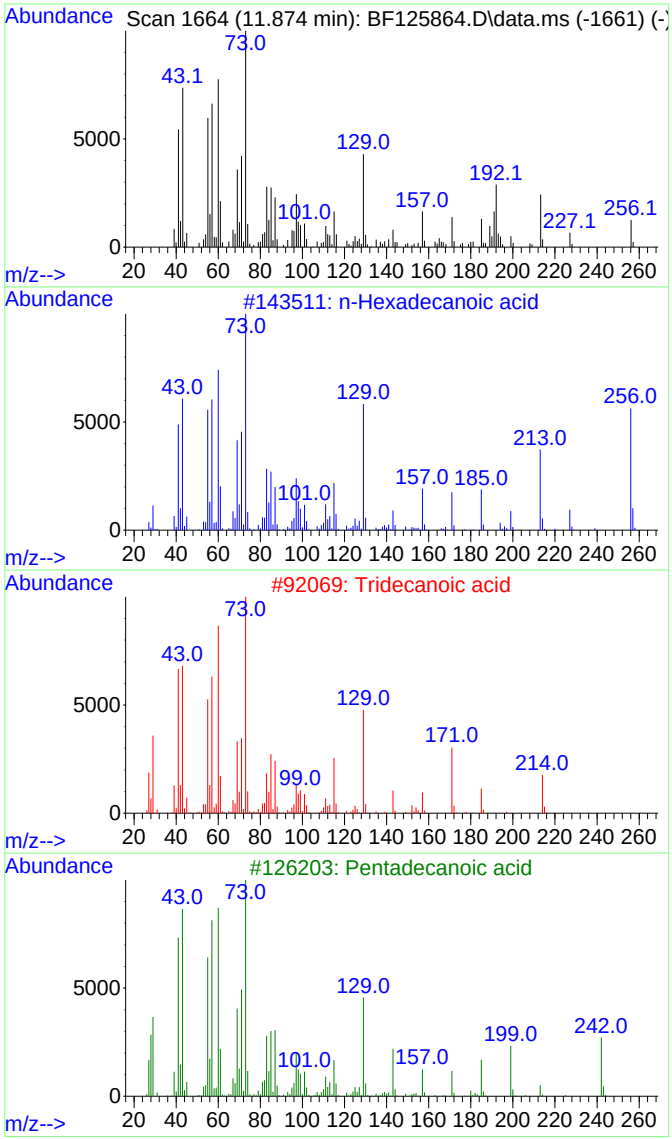
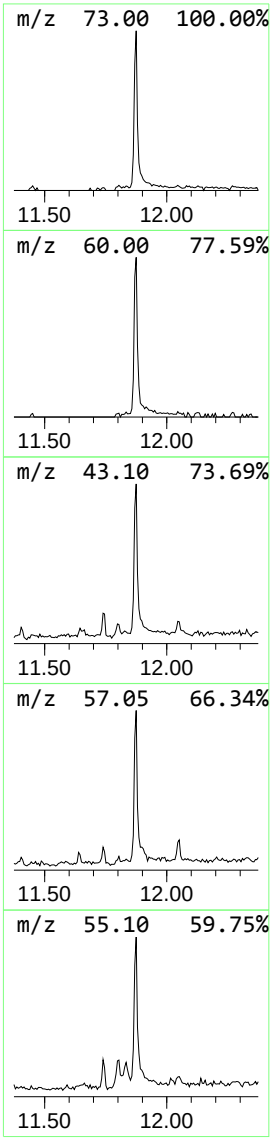
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	4.33 ng	255367	Phenanthrene-d10	11.345

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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ClientSampleId :
OR-03-101421

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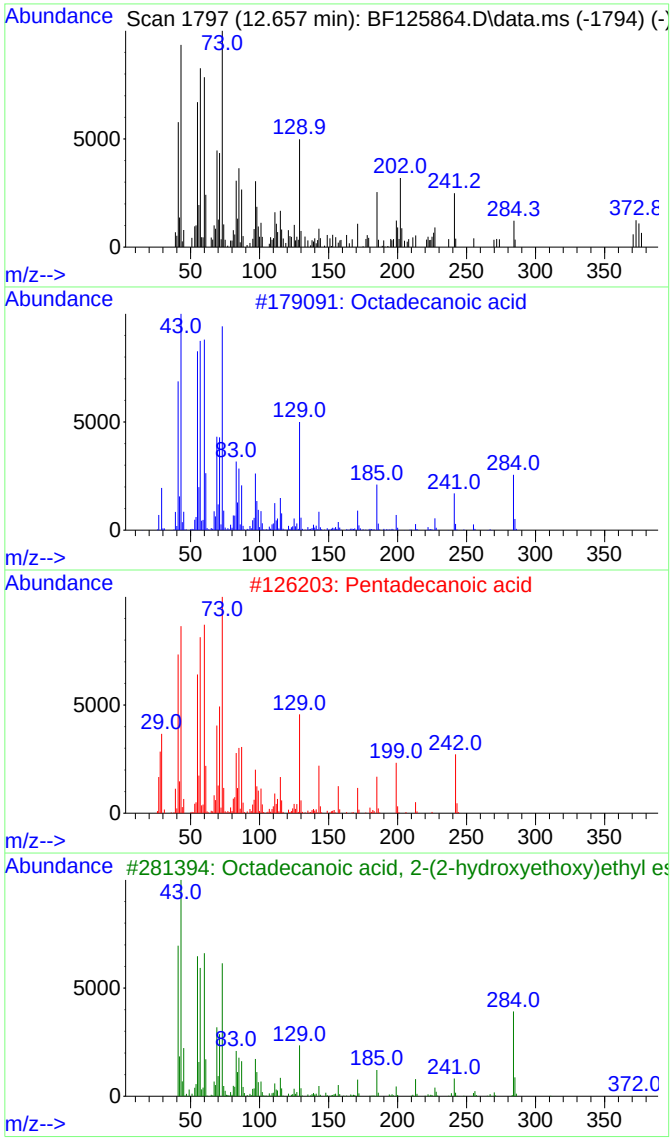
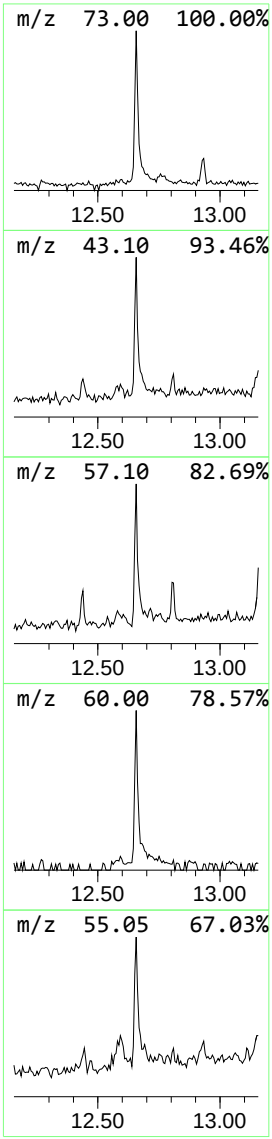
Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	3.00 ng	176834	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49





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Instrument : BNA_F
ClientSampleId : OR-03-101421

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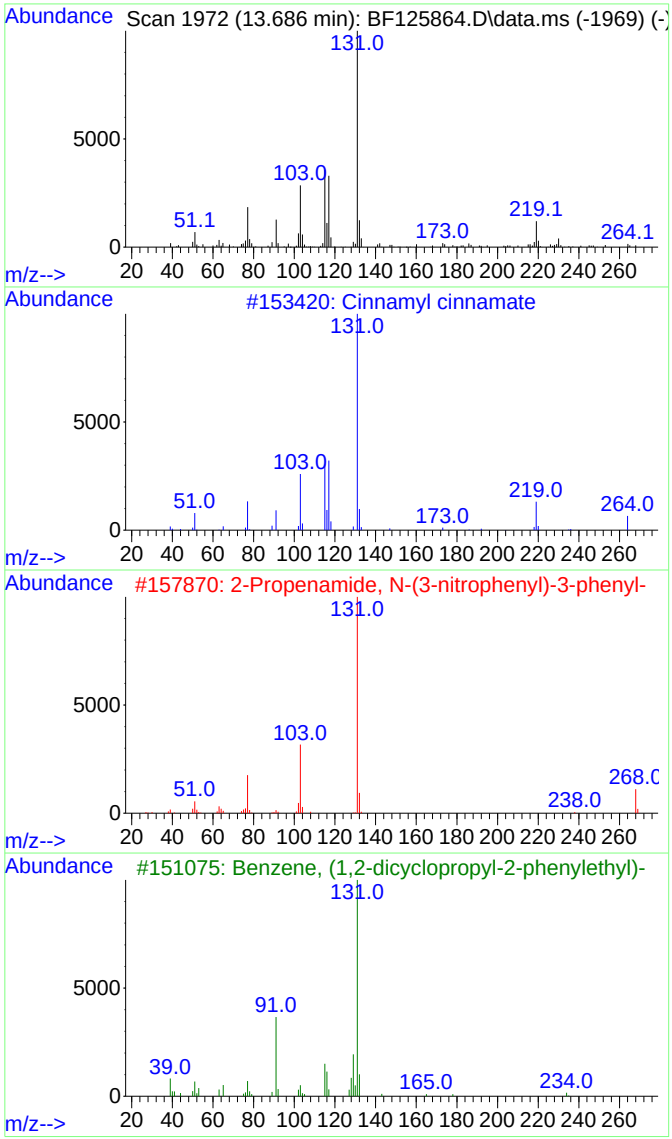
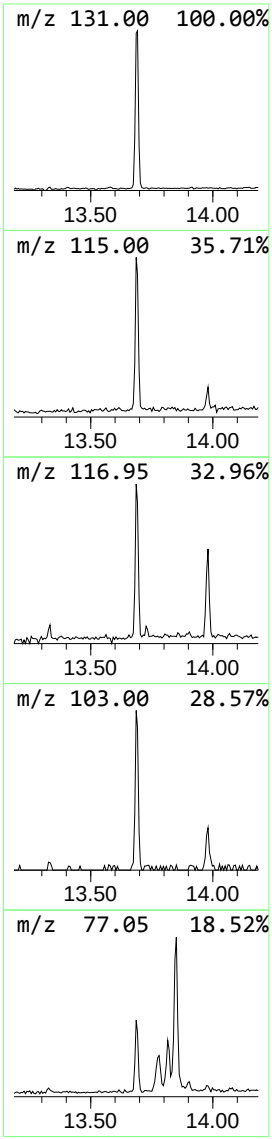
Peak Number 6 Cinnamyl cinnamate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	2.47 ng	148732	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	2-Propenamide, N-(3-nitrophenyl)...	268	C15H12N2O3	055000-38-9	53
3	Benzene, (1,2-dicyclopropyl-2-ph...	262	C20H22	110330-90-0	50
4	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	49
5	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49





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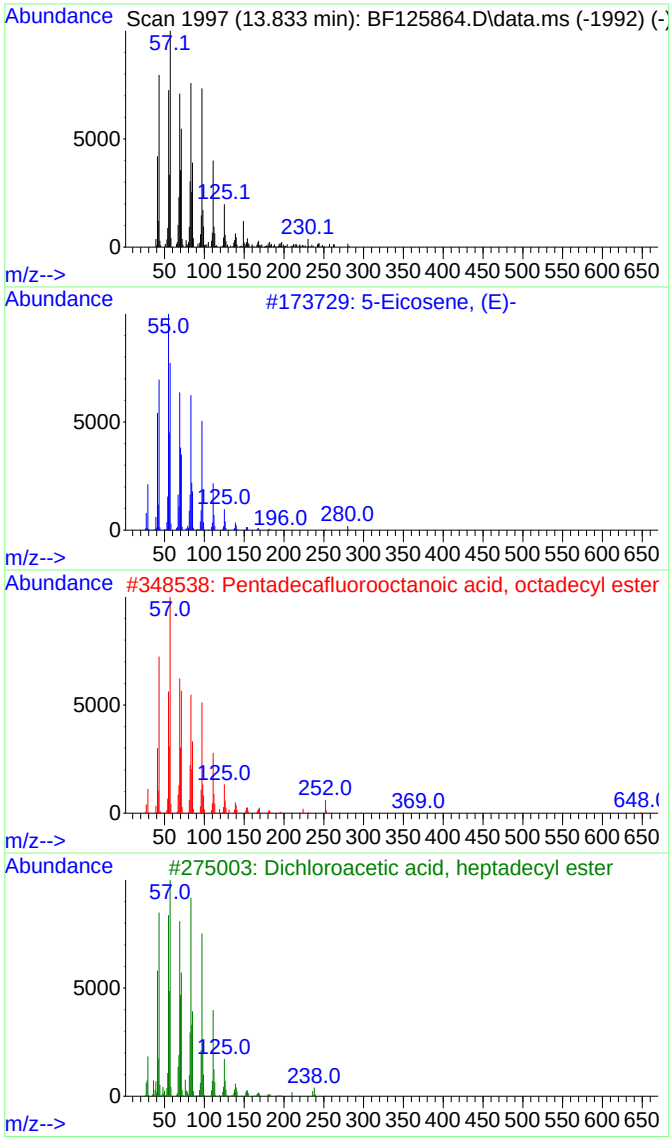
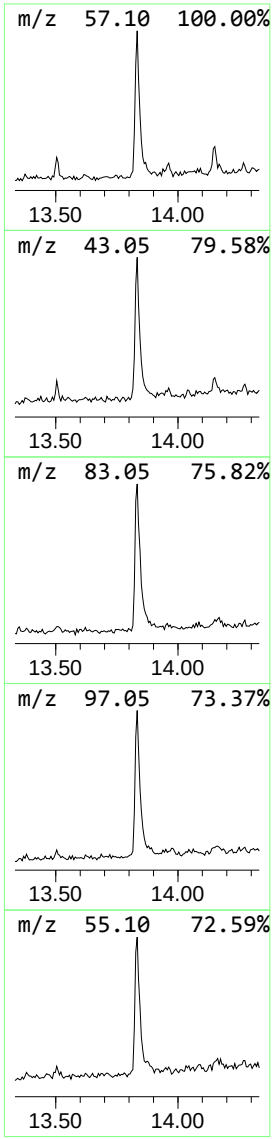
Peak Number 7 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	6.36 ng	383511	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





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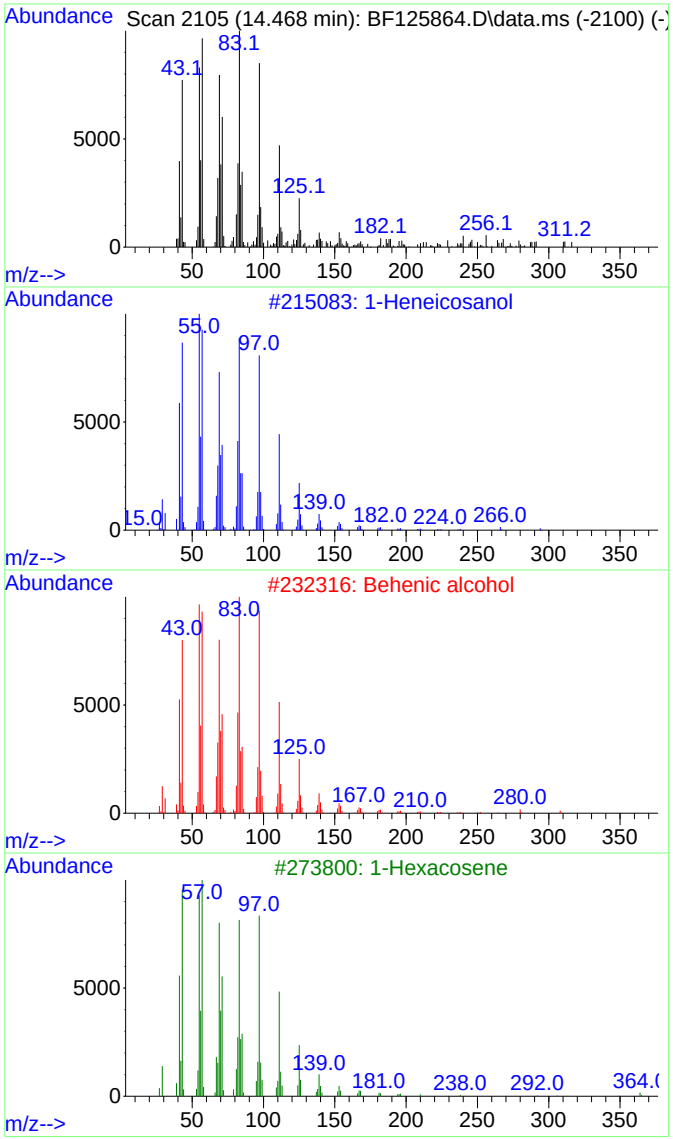
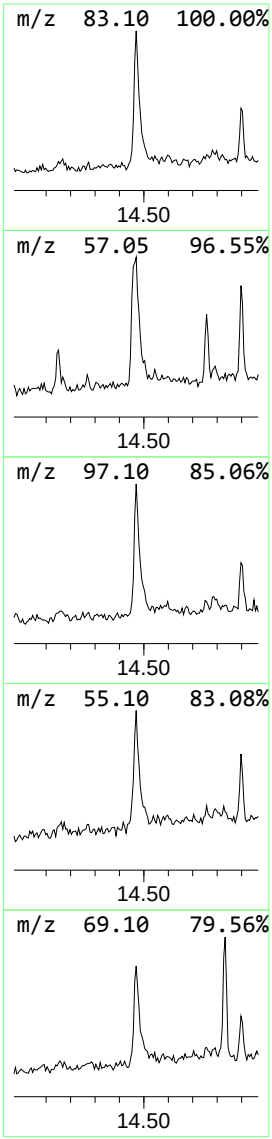
Peak Number 8 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	6.55 ng	394898	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





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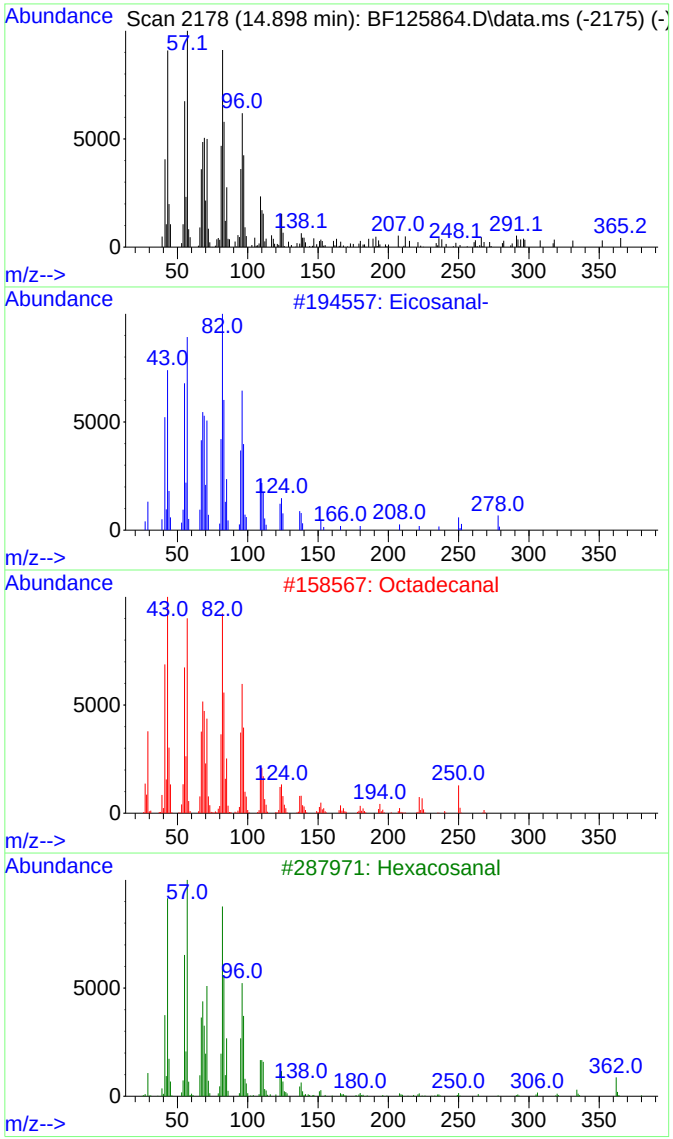
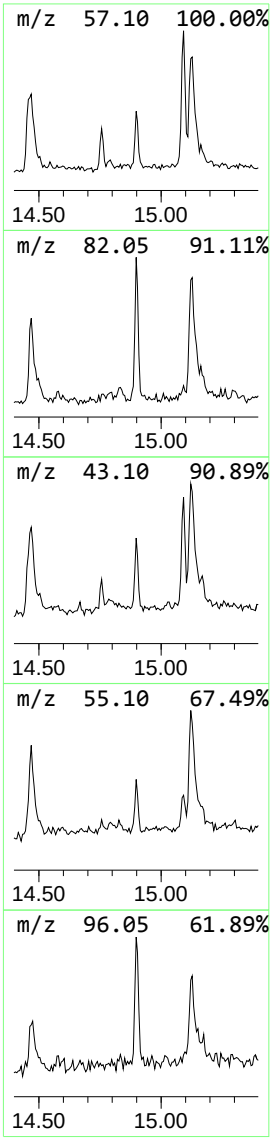
Peak Number 9 Eicosanal- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.21 ng	121664	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanal-	296	C20H40O	002400-66-0	95
2	Octadecanal	268	C18H36O	000638-66-4	94
3	Hexacosanal	380	C26H52O	026627-85-0	91
4	Tetracosanal	352	C24H48O	057866-08-7	91
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90





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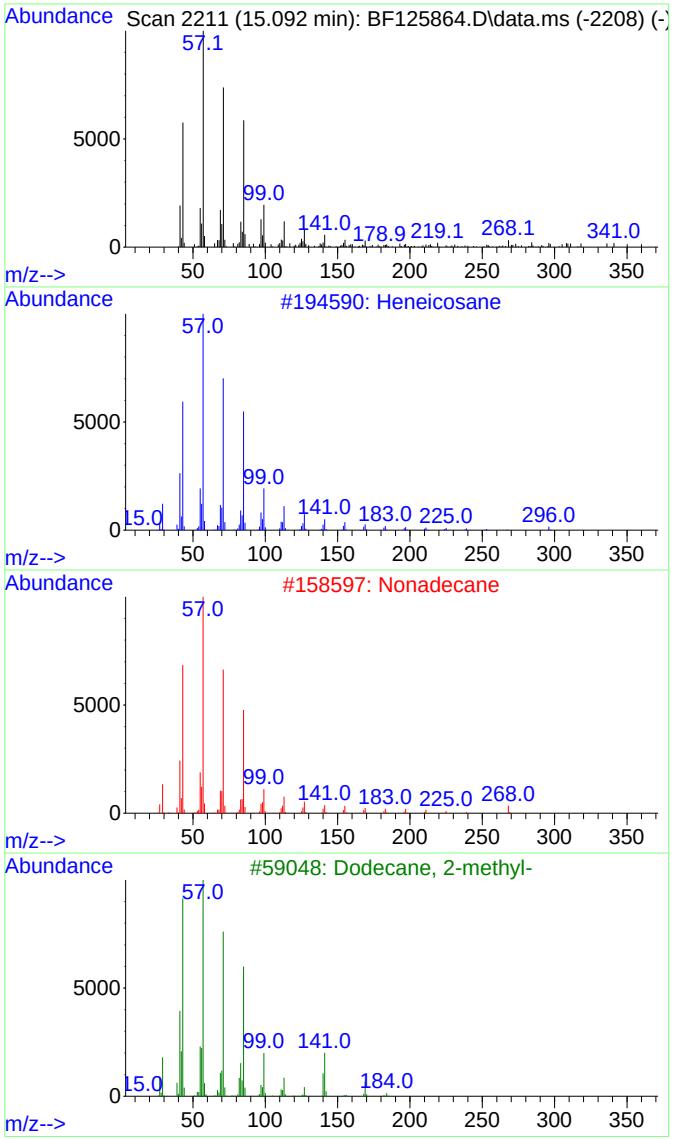
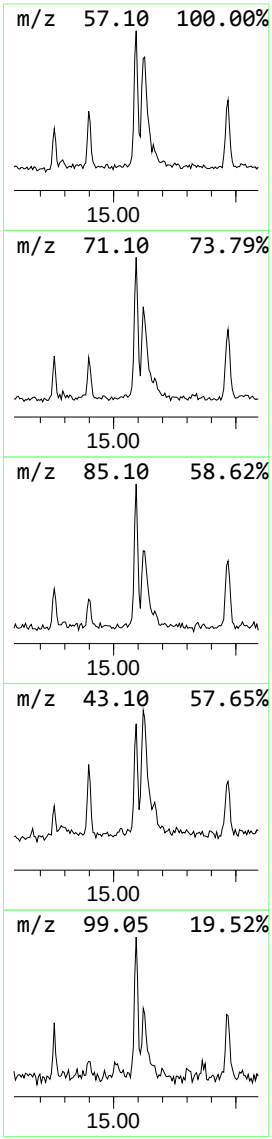
Peak Number 10 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.28 ng	125299	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Nonadecane	268	C19H40	000629-92-5	91
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87





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Data File : BF125864.D
Acq On : 15 Oct 2021 15:54
Operator : JU/CG
Sample : M4240-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-03-101421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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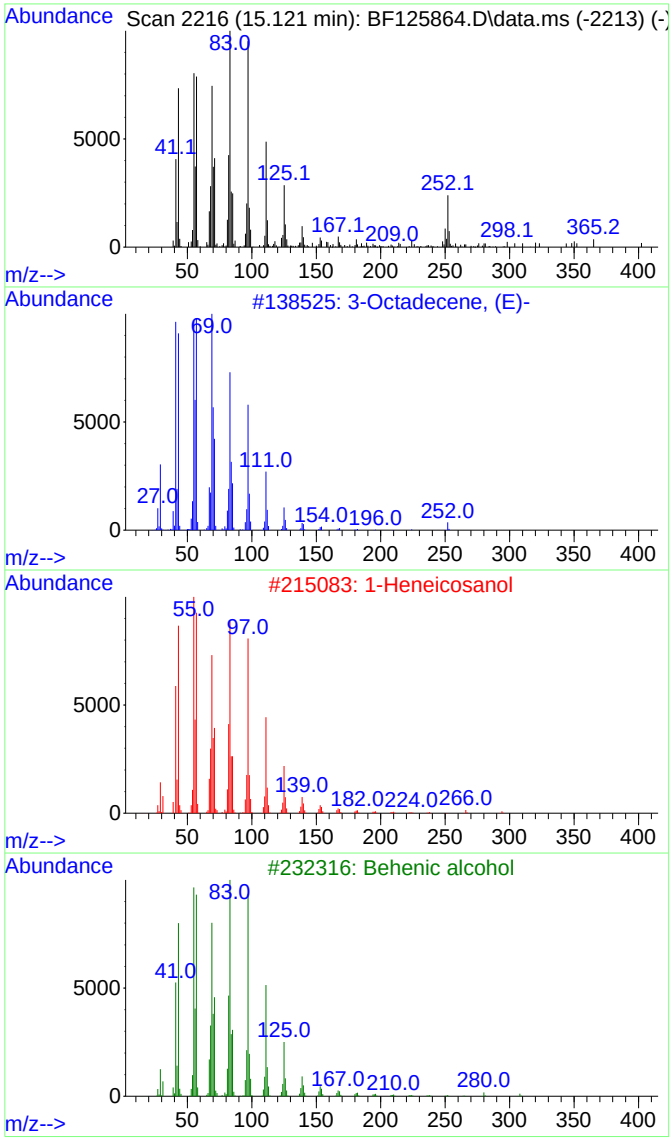
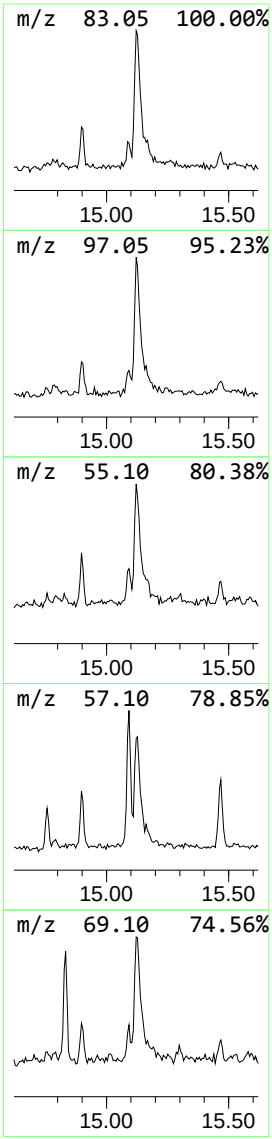
Peak Number 11 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	5.73 ng	315462	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	91





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Data File : BF125864.D
Acq On : 15 Oct 2021 15:54
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Instrument : BNA_F
ClientSampleId : OR-03-101421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
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TIC Integration Parameters: LSCINT.P

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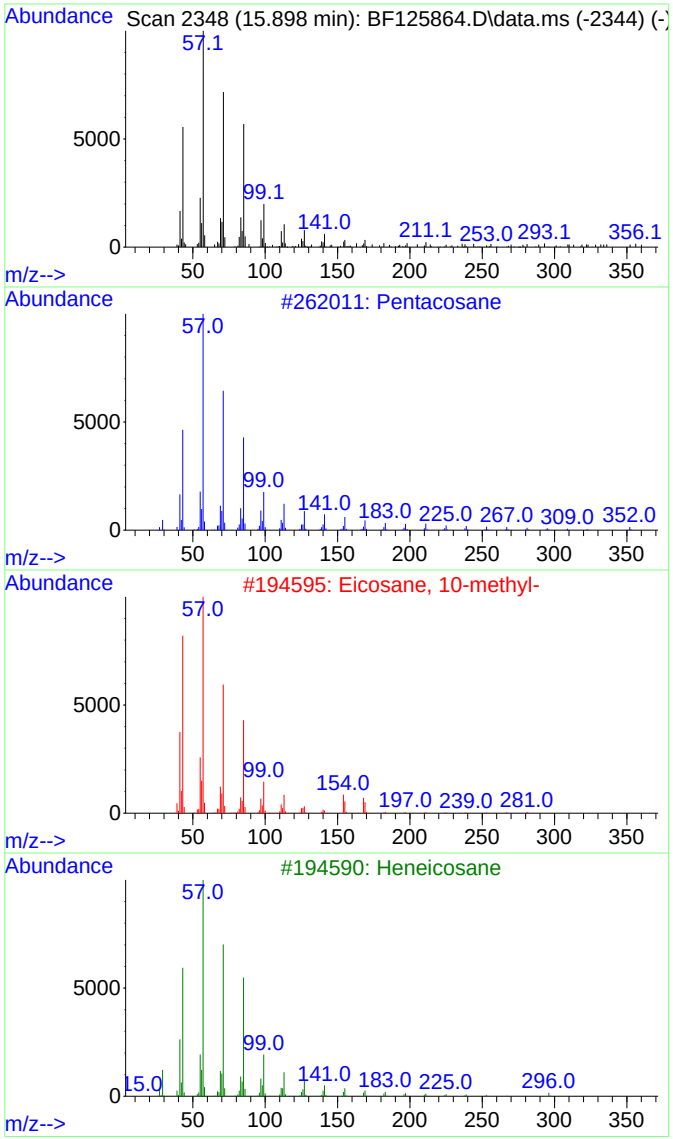
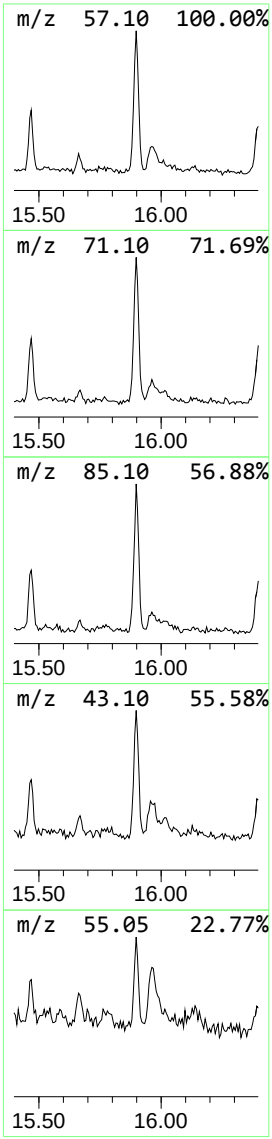
Peak Number 12 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	3.79 ng	208464	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125864.D
Acq On : 15 Oct 2021 15:54
Operator : JU/CG
Sample : M4240-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-03-101421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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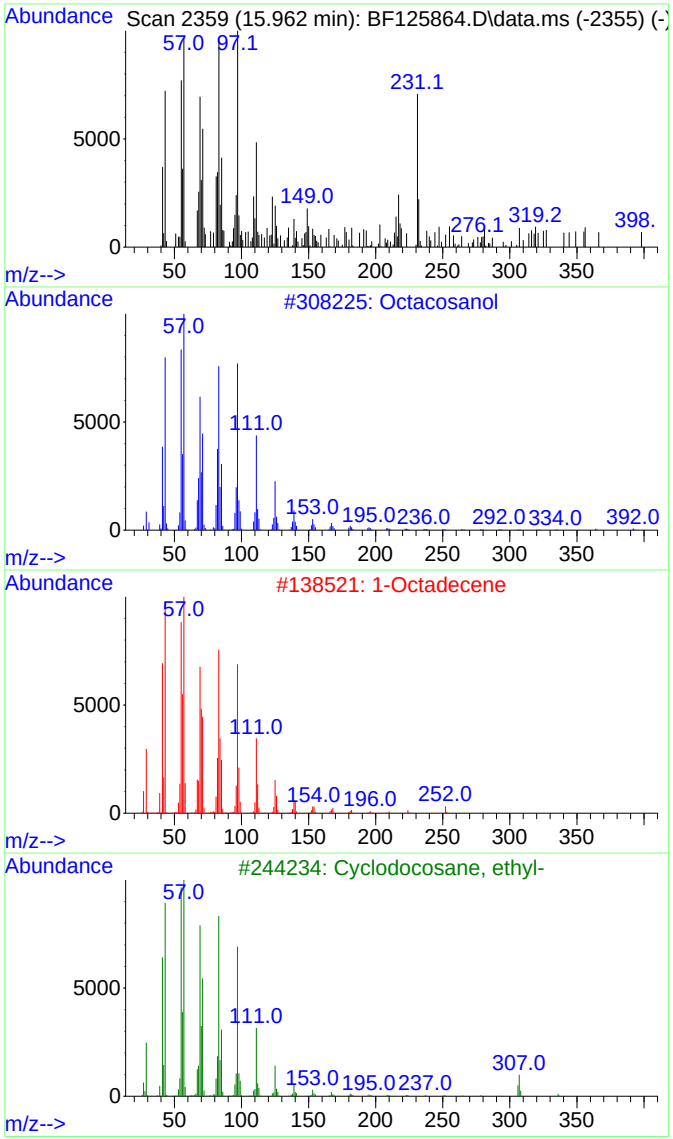
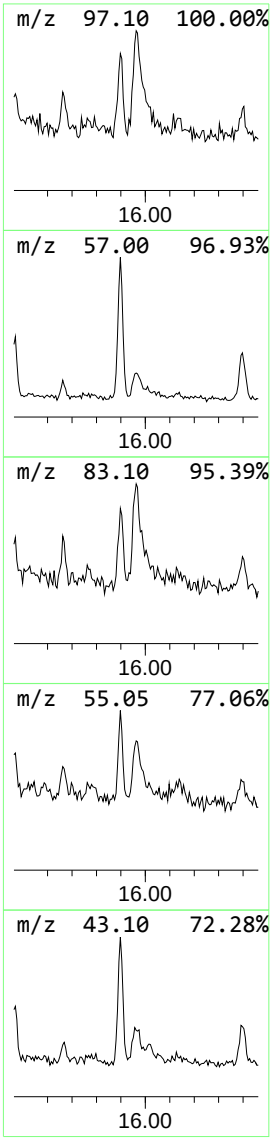
Peak Number 13 Octacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.962	2.87 ng	157749	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	86
2	1-Octadecene	252	C18H36	000112-88-9	86
3	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	70
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	70
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125864.D
Acq On : 15 Oct 2021 15:54
Operator : JU/CG
Sample : M4240-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-03-101421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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...	2.146	40.9	ng	2021550	1	6.833	989845	20.0
Ethanol, 2-(2-b...	8.016	9.3	ng	623750	2	8.116	1338580	20.0
n-Hexadecanoic ...	11.874	4.3	ng	255367	4	11.345	1180350	20.0
Octadecanoic acid	12.657	3.0	ng	176834	4	11.345	1180350	20.0
Cinnamyl cinnamate	13.686	2.5	ng	148732	5	13.980	1205170	20.0
5-Eicosene, (E)-	13.833	6.4	ng	383511	5	13.980	1205170	20.0
1-Heneicosanol	14.468	6.5	ng	394898	5	13.980	1205170	20.0
Eicosanal-	14.898	2.2	ng	121664	6	15.433	1101190	20.0
Heneicosane	15.092	2.3	ng	125299	6	15.433	1101190	20.0
3-Octadecene, (E)-	15.121	5.7	ng	315462	6	15.433	1101190	20.0
Pentacosane	15.898	3.8	ng	208464	6	15.433	1101190	20.0
Octacosanol	15.962	2.9	ng	157749	6	15.433	1101190	20.0