LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135356.D
Acq On : 20 Sep 2023 14:30
Operator : CG\JU
Sample : 04351-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPT102-01

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	490	494	506	rVB	73338	97654	3.47%	0.466%
2	5.393	557	562	578	rBV	2769324	2814961	99.91%	13.422%
3	6.034	667	671	674	rVB	266928	228993	8.13%	1.092%
4	6.404	729	734	741	rBV	2652831	2817536	100.00%	13.434%
5	6.757	790	794	803	rVV	1040033	829548	29.44%	3.955%
6	6.828	803	806	810	rVV	72099	66319	2.35%	0.316%
7	6.869	810	813	818	rVB	35640	30247	1.07%	0.144%
8	7.322	885	890	893	rBV	1993380	1785814	63.38%	8.515%
9	8.034	1007	1011	1015	rBV	1226478	1052177	37.34%	5.017%
10	9.116	1190	1195	1198	rBV	3149715	2798804	99.34%	13.345%
11	9.234	1211	1215	1219	rBV	37770	39893	1.42%	0.190%
12	9.792	1306	1310	1322	rVB	1325497	1113451	39.52%	5.309%
13	10.586	1441	1445	1461	rBV	1546911	1497394	53.15%	7.140%
14	11.280	1560	1563	1567	rBV	1072669	1011675	35.91%	4.824%
15	11.351	1570	1575	1581	rVB5	33163	37882	1.34%	0.181%
16	11.822	1651	1655	1663	rBV2	125703	161580	5.73%	0.770%
17	12.610	1786	1789	1795	rBV5	25696	44663	1.59%	0.213%
18	12.880	1831	1835	1838	rBV	1959562	1744520	61.92%	8.318%
19	13.116	1872	1875	1878	rBV	45905	40171	1.43%	0.192%
20	13.369	1913	1918	1924	rBV	599710	569410	20.21%	2.715%
21	13.457	1929	1933	1936	rVV2	59757	66922	2.38%	0.319%
22	13.792	1987	1990	1993	rBV	70944	58700	2.08%	0.280%
23	13.939	2011	2015	2019	rBV	716895	649250	23.04%	3.096%
24	14.110	2041	2044	2047	rVB	95741	80482	2.86%	0.384%
25	14.416	2093	2096	2099	rBV	95523	87806	3.12%	0.419%
26	14.721	2145	2148	2153	rBV	107493	110072	3.91%	0.525%
27	15.057	2202	2205	2210	rVB	99029	116855	4.15%	0.557%
28	15.410	2260	2265	2268	rBV	656126	776557	27.56%	3.703%
29	15.874	2341	2344	2349	rBV	88417	122885	4.36%	0.586%
30	16.392	2428	2432	2437	rVB3	75332	120854	4.29%	0.576%

Sum of corrected areas: 20973075

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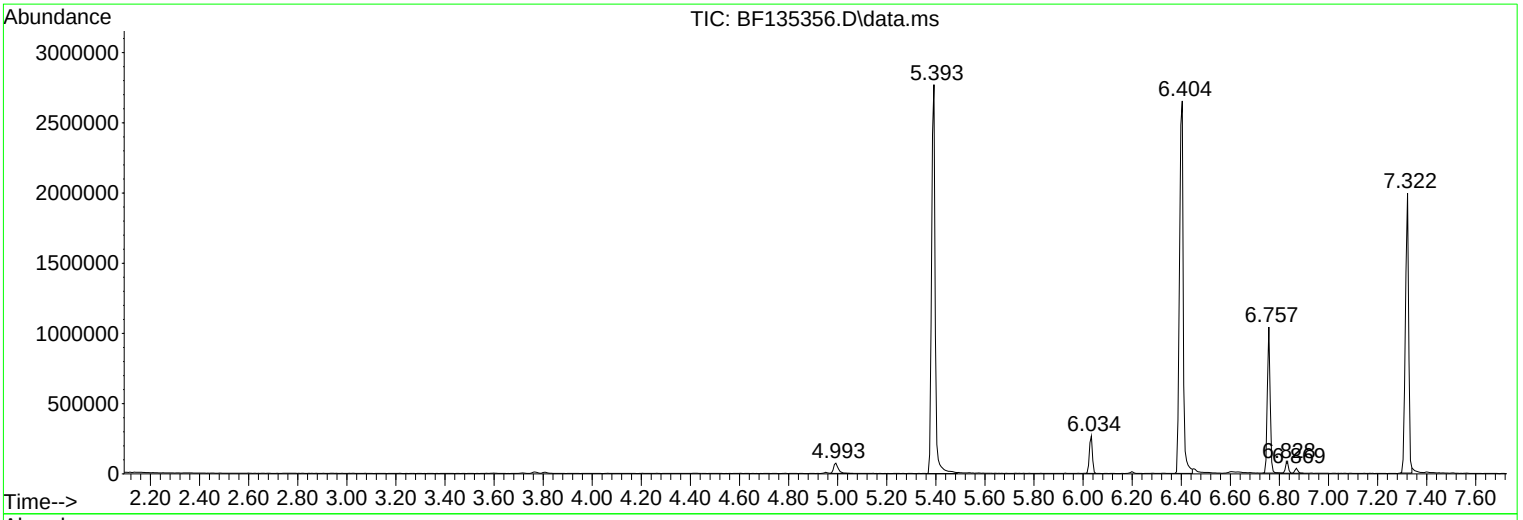
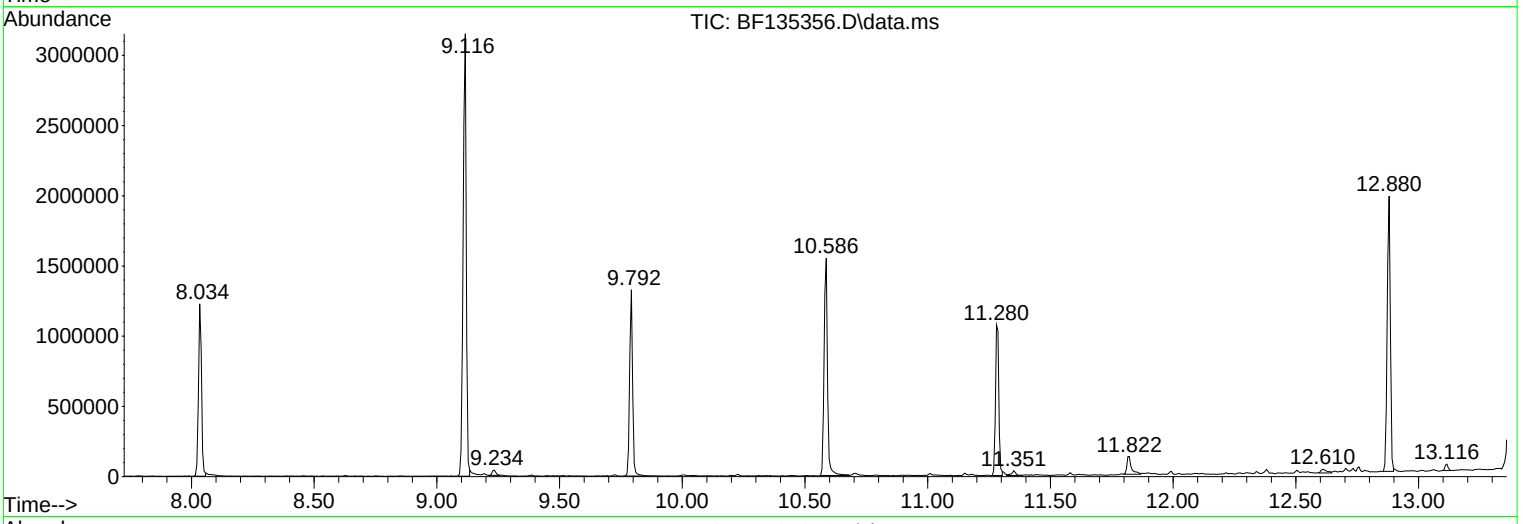
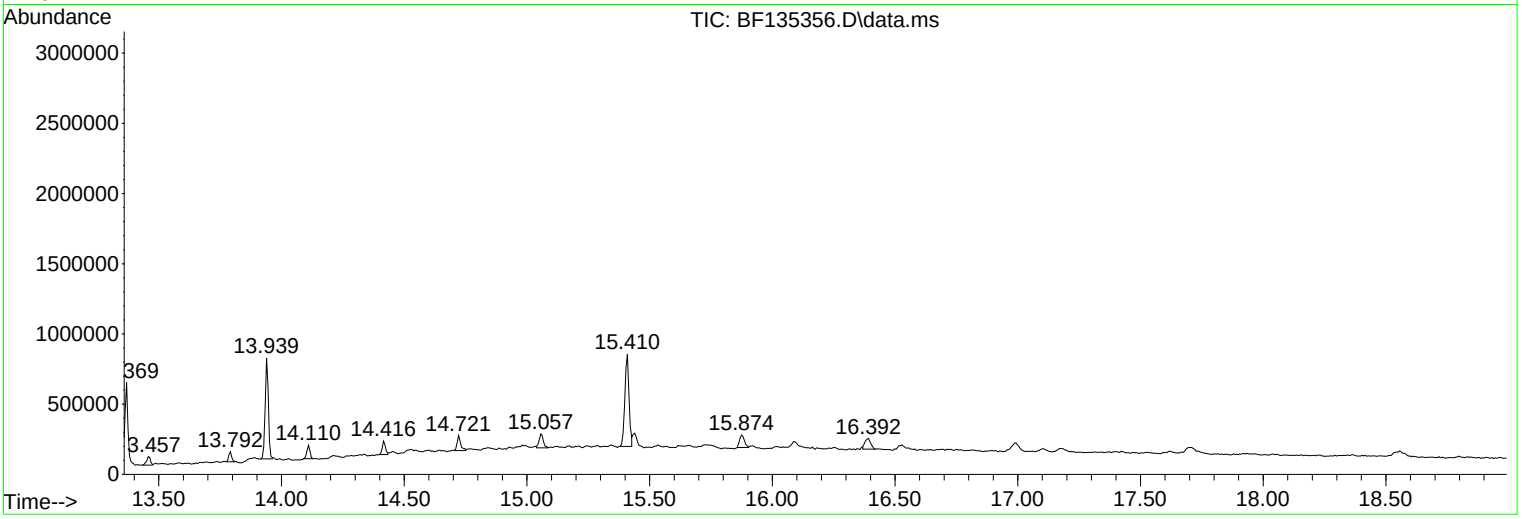
ClientSampleId :
CPT102-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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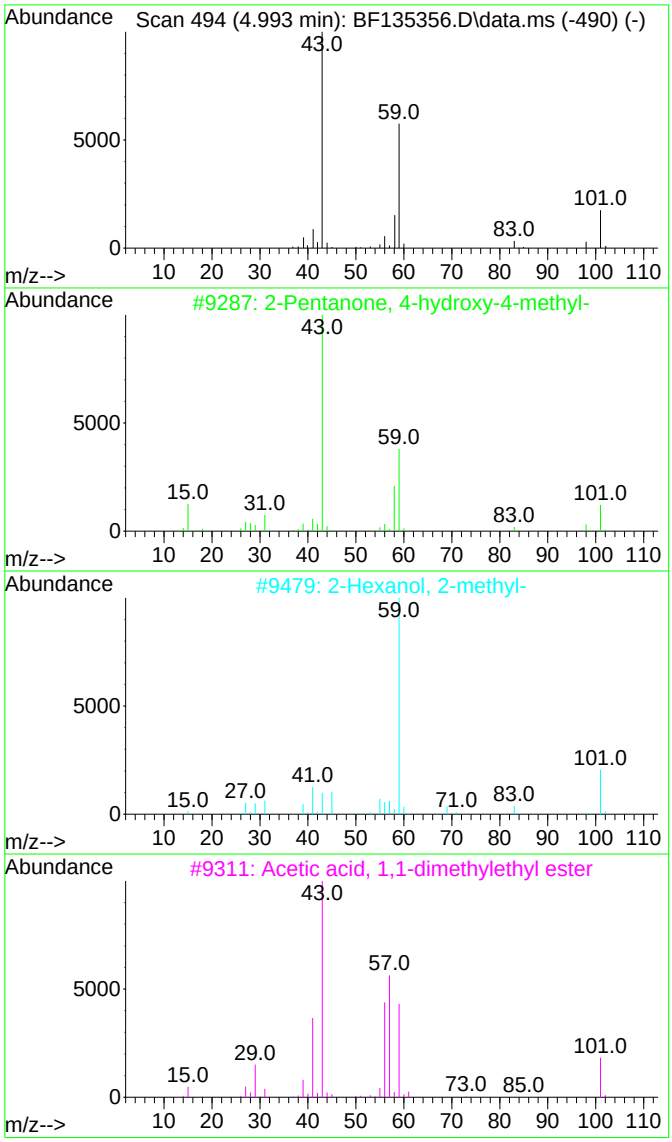
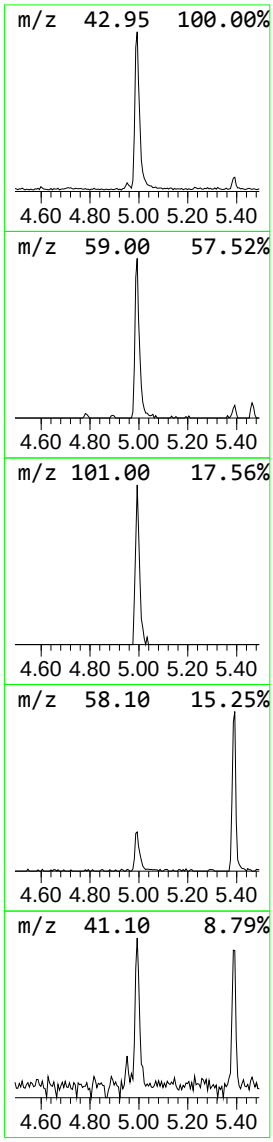
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	2.35 ng	97654	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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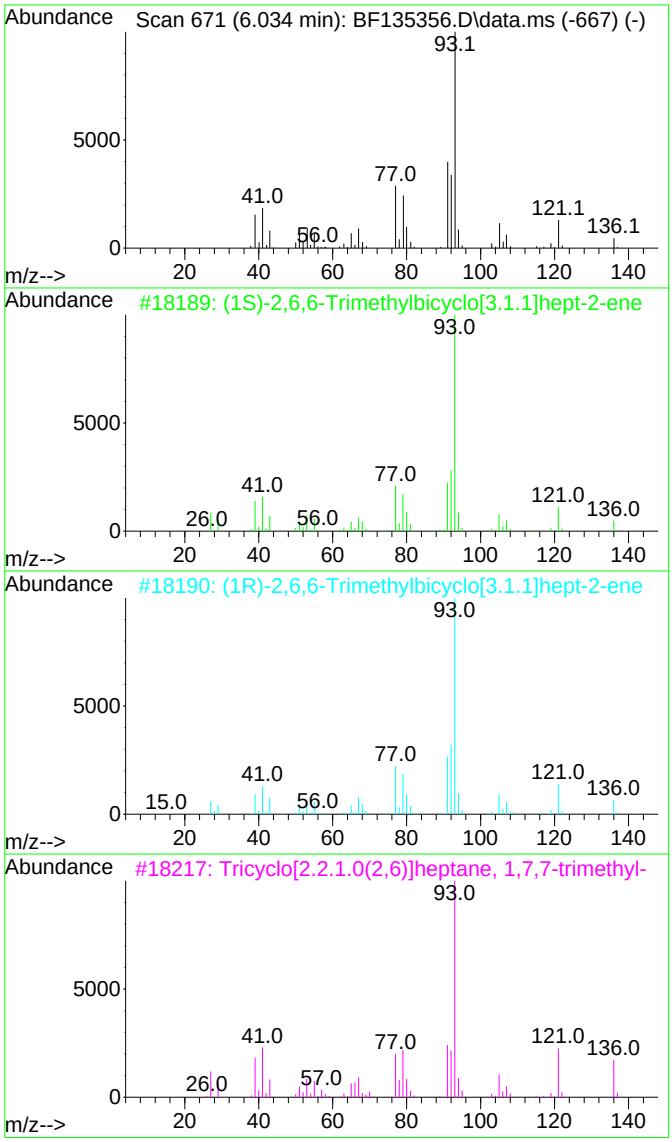
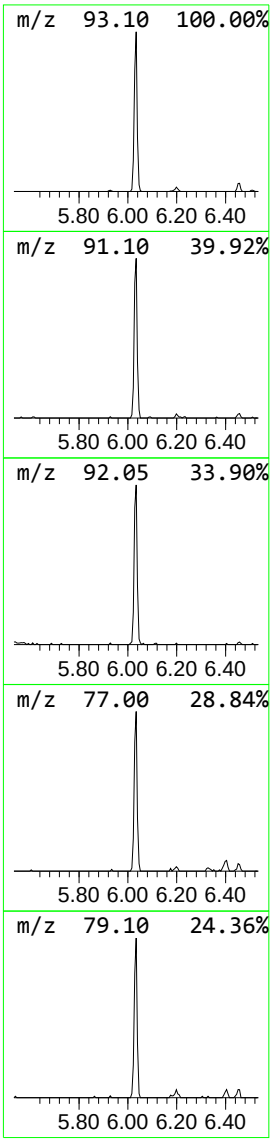
****
Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.034	5.52 ng	228993	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	94
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	.alpha.-Pinene	136	C10H16	000080-56-8	91
5	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91





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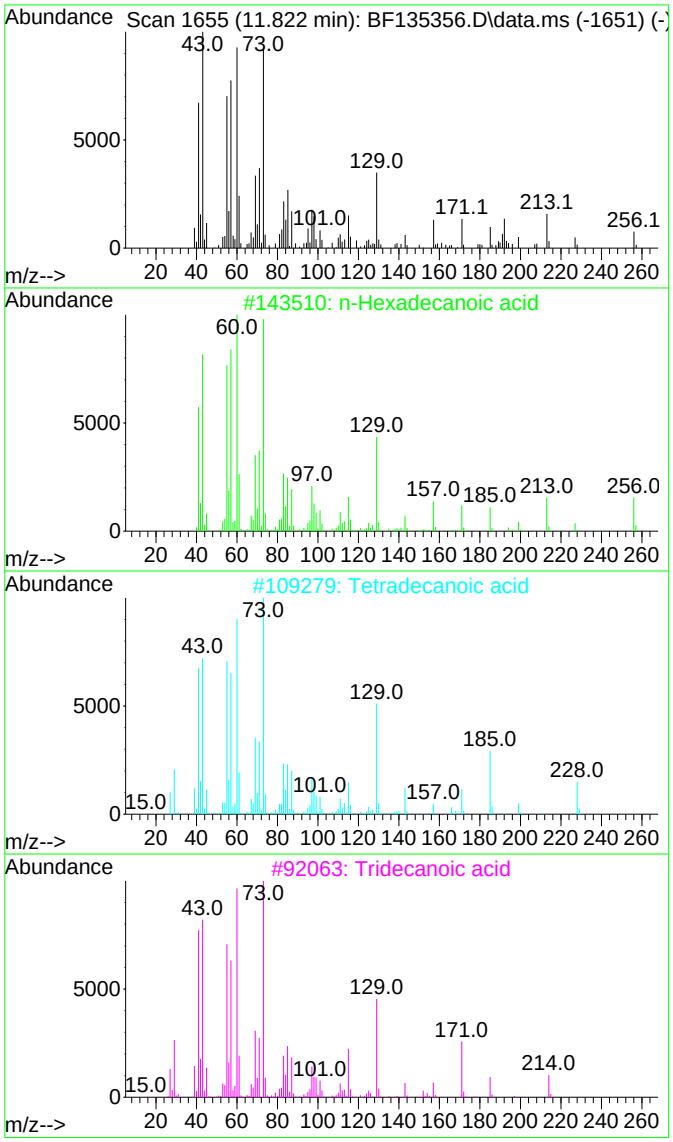
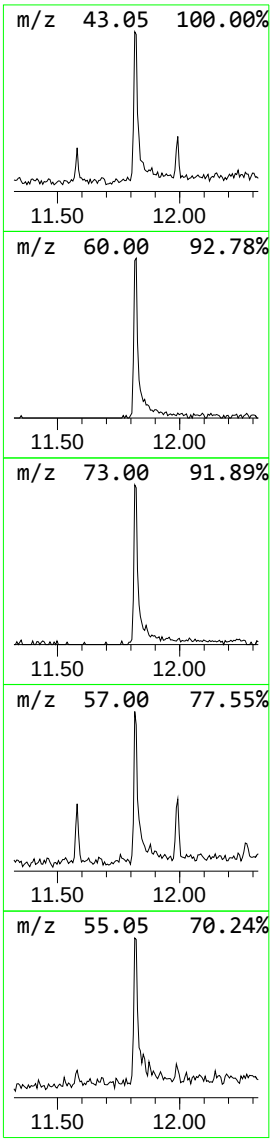
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	3.19 ng	161580	Phenanthrene-d10	11.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	78





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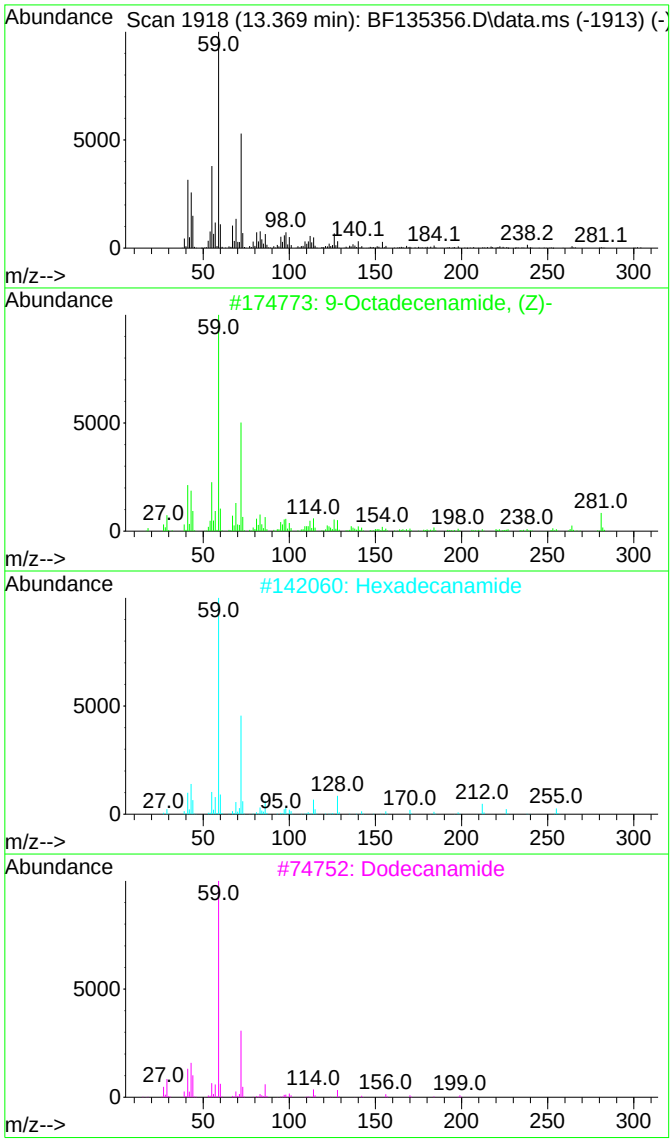
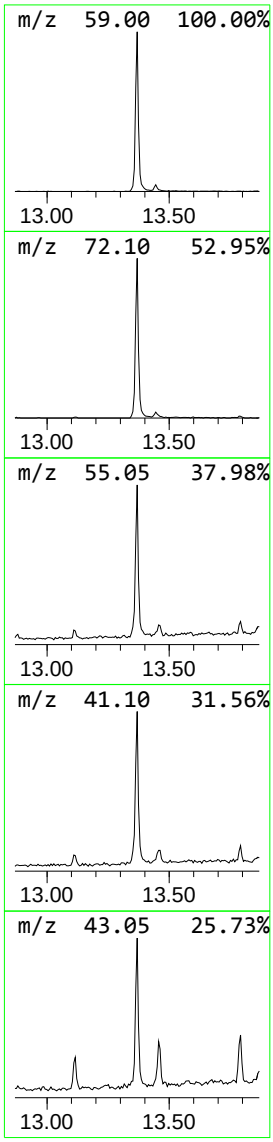
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	17.54 ng	569410	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Hexadecanamide	255	C16H33NO	000629-54-9	56
3	Dodecanamide	199	C12H25NO	001120-16-7	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	50





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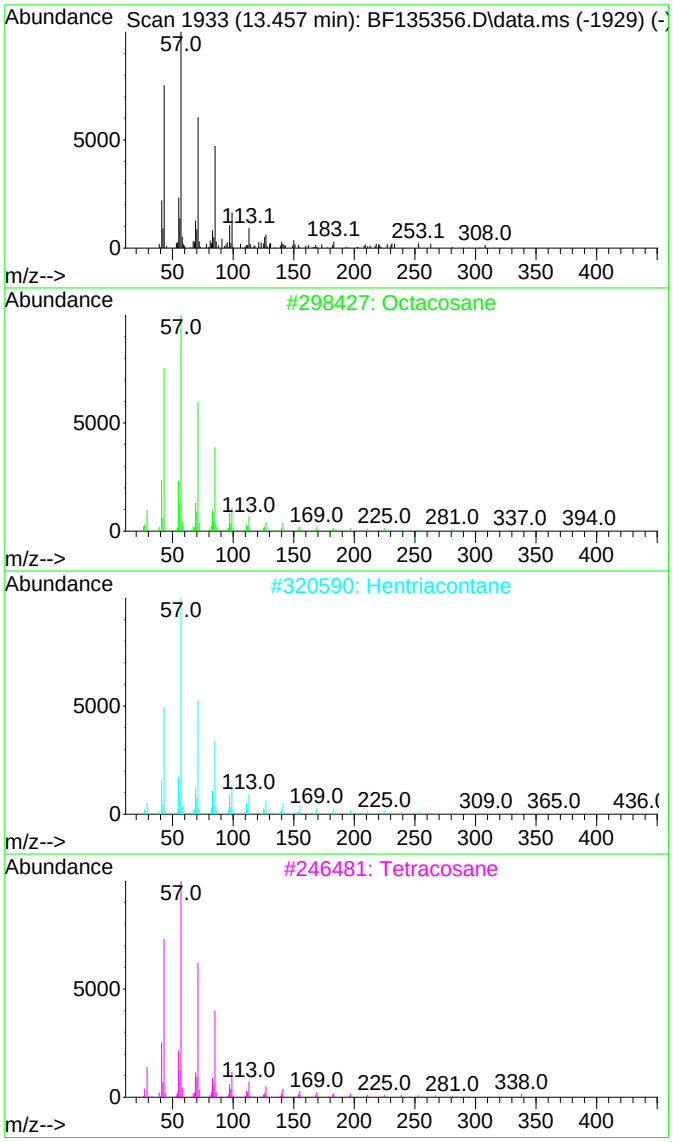
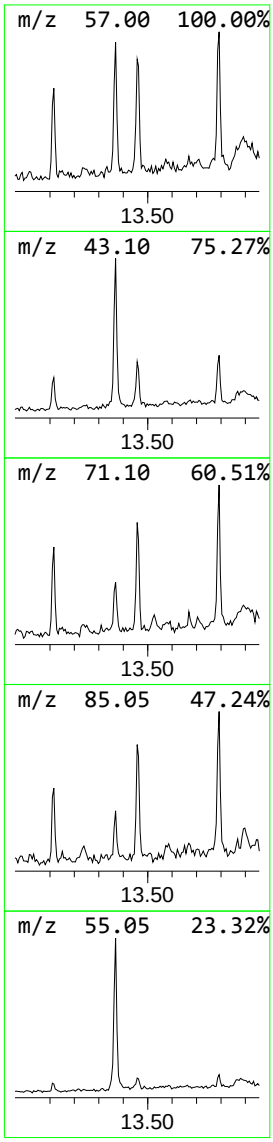
Peak Number 5 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	2.06 ng	66922	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Hentriacontane	437	C31H64	000630-04-6	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86





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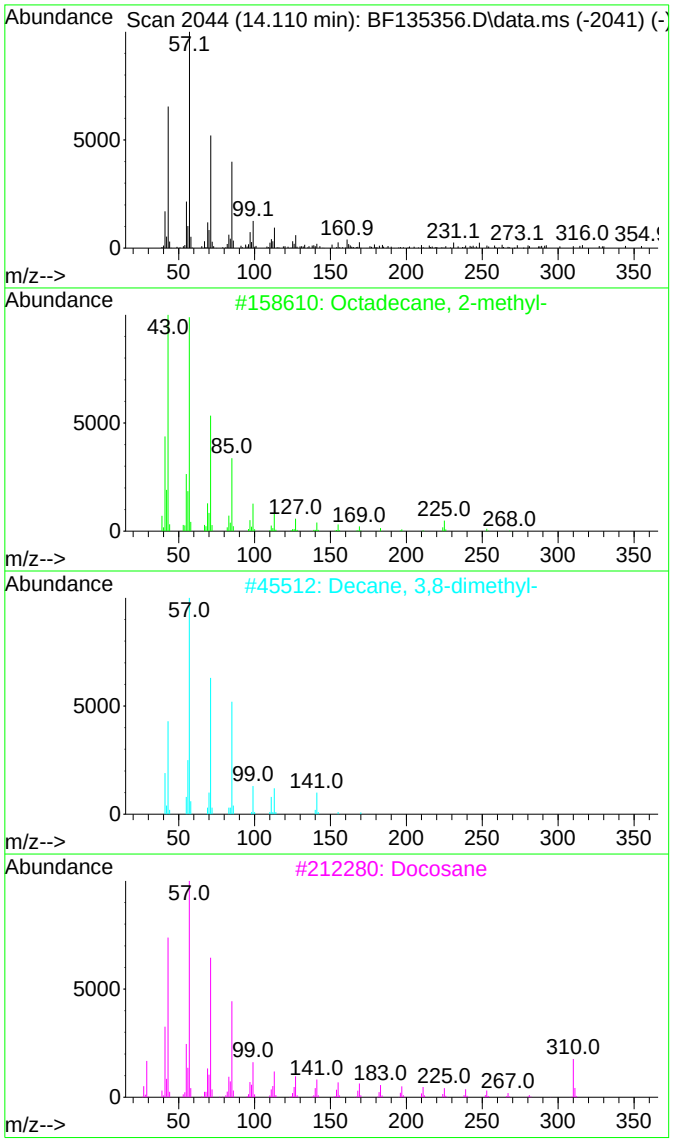
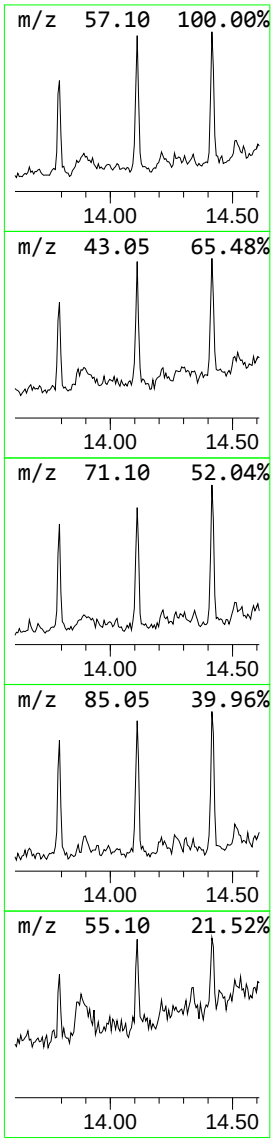
Peak Number 6 Octadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.48 ng	80482	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90
3	Docosane	310	C22H46	000629-97-0	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Tetracosane	338	C24H50	000646-31-1	87





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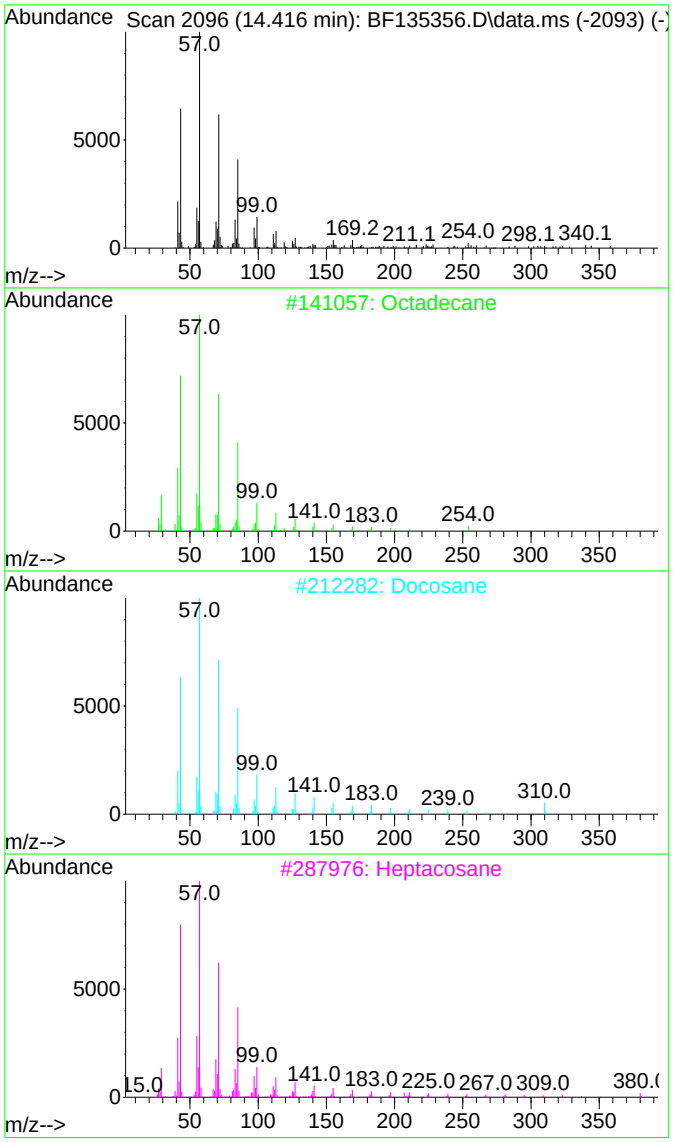
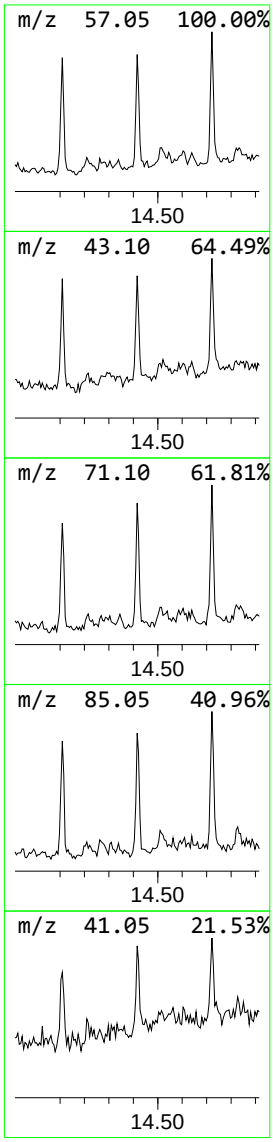
Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	2.70 ng	87806	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Docosane	310	C22H46	000629-97-0	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Hentriacontane	437	C31H64	000630-04-6	90





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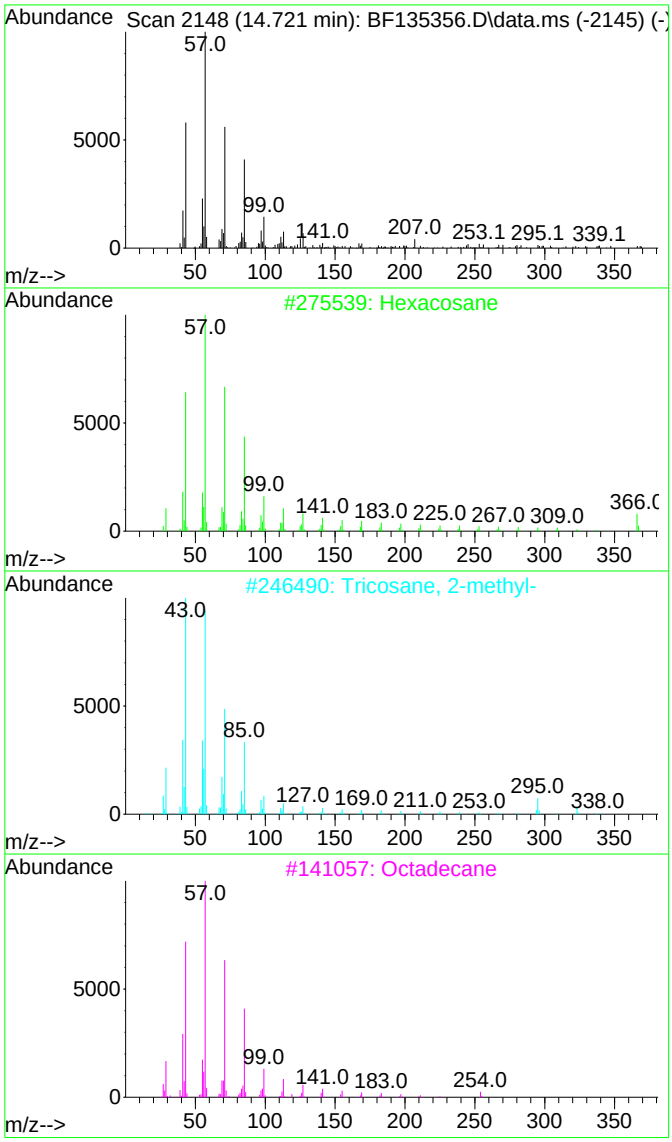
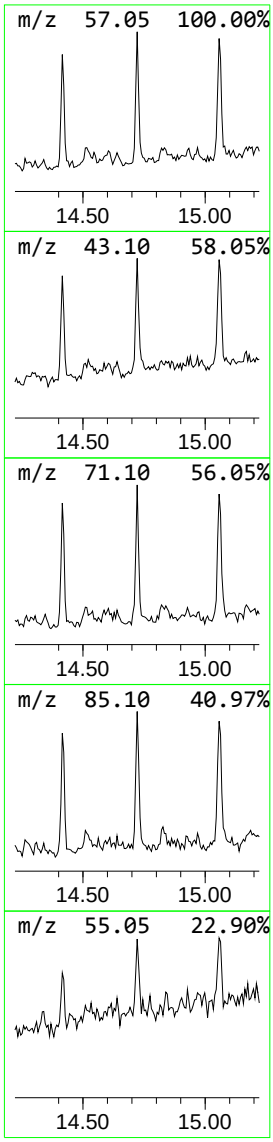
Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.83 ng	110072	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	86
3	Octadecane	254	C18H38	000593-45-3	80
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80





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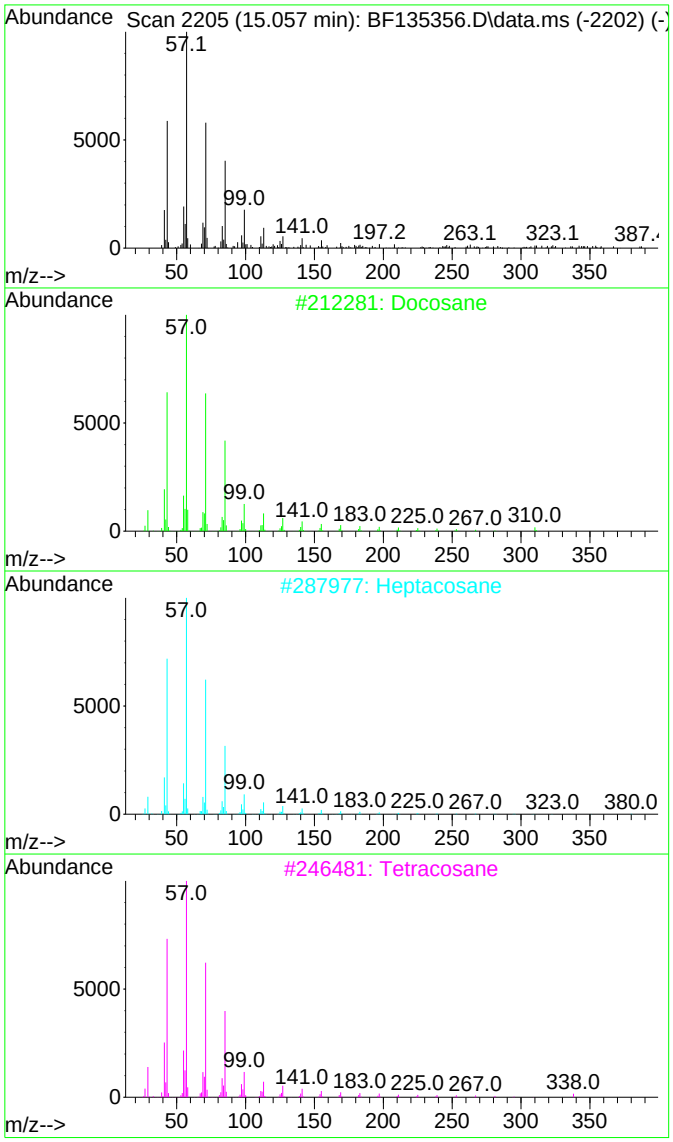
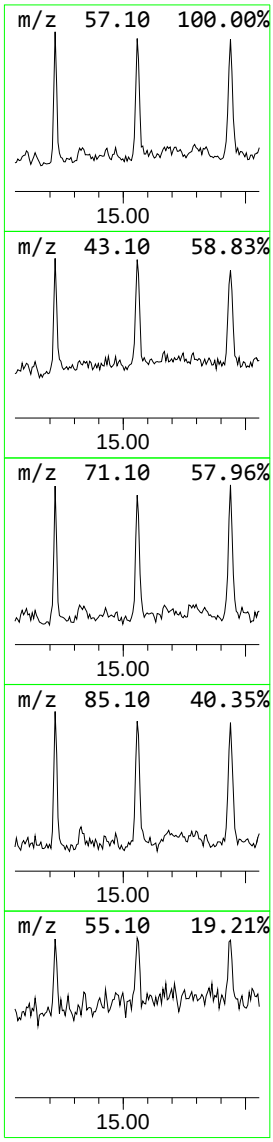
Peak Number 9 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	3.01 ng	116855	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Tricosane	324	C23H48	000638-67-5	90
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135356.D
Acq On : 20 Sep 2023 14:30
Operator : CG\JU
Sample : 04351-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPT102-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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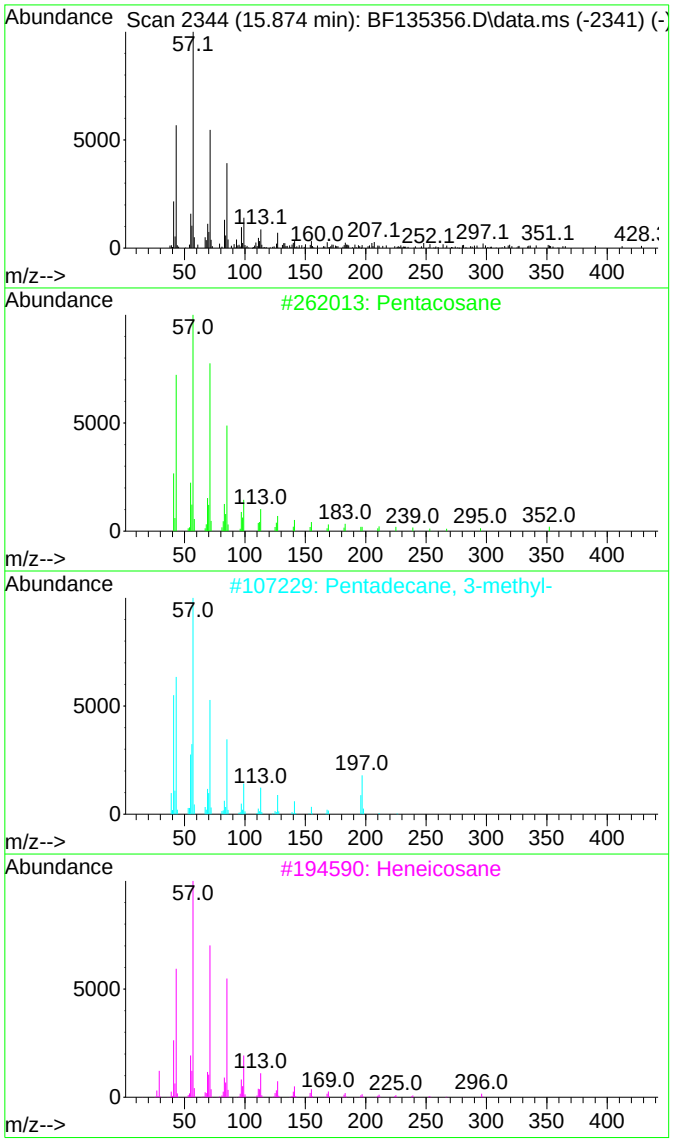
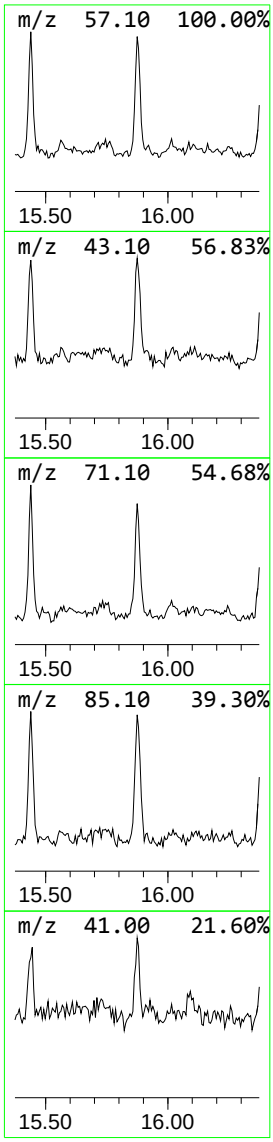
Peak Number 10 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	3.16 ng	122885	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	94
2	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
5	Nonadecane	268	C19H40	000629-92-5	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135356.D
Acq On : 20 Sep 2023 14:30
Operator : CG\JU
Sample : 04351-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPT102-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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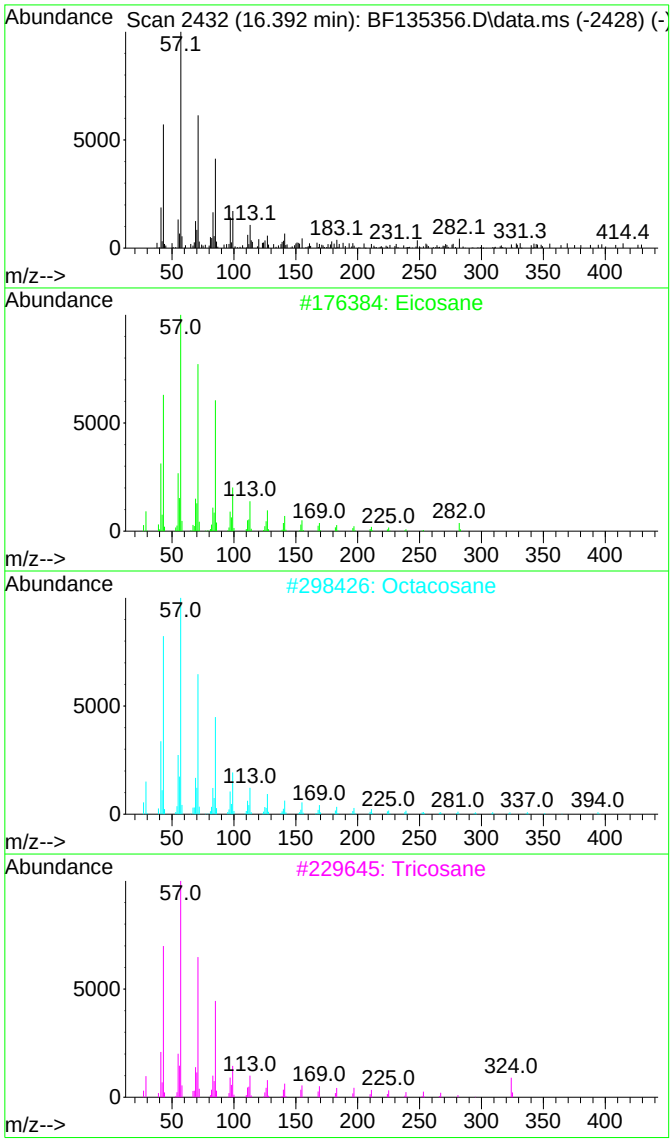
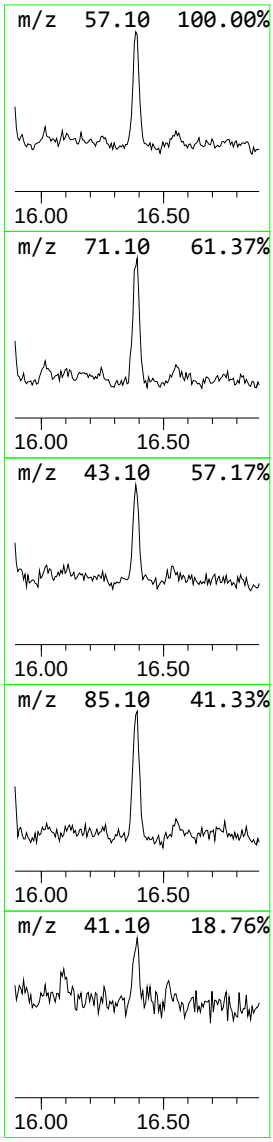
Peak Number 11 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	3.11 ng	120854	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octacosane	394	C28H58	000630-02-4	76
3	Tricosane	324	C23H48	000638-67-5	76
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	76
5	Behenyl chloride	344	C22H45Cl	042217-03-8	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135356.D
Acq On : 20 Sep 2023 14:30
Operator : CG\JU
Sample : 04351-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPT102-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
2-Pentanone, 4-...	4.993	2.4	ng	97654	1	6.757	829548	20.0
(1S)-2,6,6-Trim...	6.034	5.5	ng	228993	1	6.757	829548	20.0
n-Hexadecanoic ...	11.822	3.2	ng	161580	4	11.286	1011680	20.0
9-Octadecenamid...	13.368	17.5	ng	569410	5	13.939	649250	20.0
Octacosane	13.457	2.1	ng	66922	5	13.939	649250	20.0
Octadecane, 2-m...	14.110	2.5	ng	80482	5	13.939	649250	20.0
Octadecane	14.416	2.7	ng	87806	5	13.939	649250	20.0
Hexacosane	14.721	2.8	ng	110072	6	15.410	776557	20.0
Docosane	15.057	3.0	ng	116855	6	15.410	776557	20.0
Pentacosane	15.874	3.2	ng	122885	6	15.410	776557	20.0
Eicosane	16.392	3.1	ng	120854	6	15.410	776557	20.0