LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134108.D
Acq On : 06 Jul 2023 21:17
Operator : CG\JU
Sample : 03476-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DOREMUS-COMP-2

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	23	rVB	1352225	1787201	58.51%	6.871%
2	2.281	30	33	41	rVB	41649	57774	1.89%	0.222%
3	5.098	508	512	521	rVB	175607	238330	7.80%	0.916%
4	5.487	573	578	581	rBV	2848810	2781773	91.07%	10.695%
5	6.487	742	748	763	rBV	2515673	2929991	95.93%	11.265%
6	6.845	805	809	822	rBV	732803	595195	19.49%	2.288%
7	7.410	900	905	908	rBV	2042708	1800021	58.93%	6.921%
8	8.122	1023	1026	1034	rVB	919779	747517	24.47%	2.874%
9	9.204	1205	1210	1213	rBV	3728778	3054432	100.00%	11.744%
10	9.880	1322	1325	1329	rBV	1004475	825215	27.02%	3.173%
11	10.598	1444	1447	1456	rBV	457071	444070	14.54%	1.707%
12	10.674	1456	1460	1469	rBV	2261459	2276702	74.54%	8.754%
13	10.739	1469	1471	1477	rVB3	34892	41347	1.35%	0.159%
14	10.910	1497	1500	1504	rVB	44912	39100	1.28%	0.150%
15	11.374	1575	1579	1583	rBV	1032883	883054	28.91%	3.395%
16	11.480	1594	1597	1601	rBV2	45682	39416	1.29%	0.152%
17	11.910	1666	1670	1672	rBV	428182	377663	12.36%	1.452%
18	11.945	1672	1676	1679	rVB	1909677	1596080	52.25%	6.137%
19	12.698	1801	1804	1811	rBV	76851	94951	3.11%	0.365%
20	12.974	1846	1851	1854	rBV	3176820	2983523	97.68%	11.471%
21	13.251	1893	1898	1902	rVB	33684	37746	1.24%	0.145%
22	13.915	2007	2011	2022	rBV3	80251	190046	6.22%	0.731%
23	14.033	2028	2031	2039	rVB	666114	654647	21.43%	2.517%
24	14.145	2046	2050	2055	rBV	166515	156111	5.11%	0.600%
25	14.898	2174	2178	2182	rBV	145145	148722	4.87%	0.572%
26	15.539	2281	2287	2297	rBV	374432	524721	17.18%	2.017%
27	17.362	2591	2597	2612	rVB7	22091	79853	2.61%	0.307%
28	18.039	2702	2712	2714	rBV7	27842	75238	2.46%	0.289%
29	18.662	2807	2818	2836	rBV8	91138	548572	17.96%	2.109%

Sum of corrected areas: 26009011

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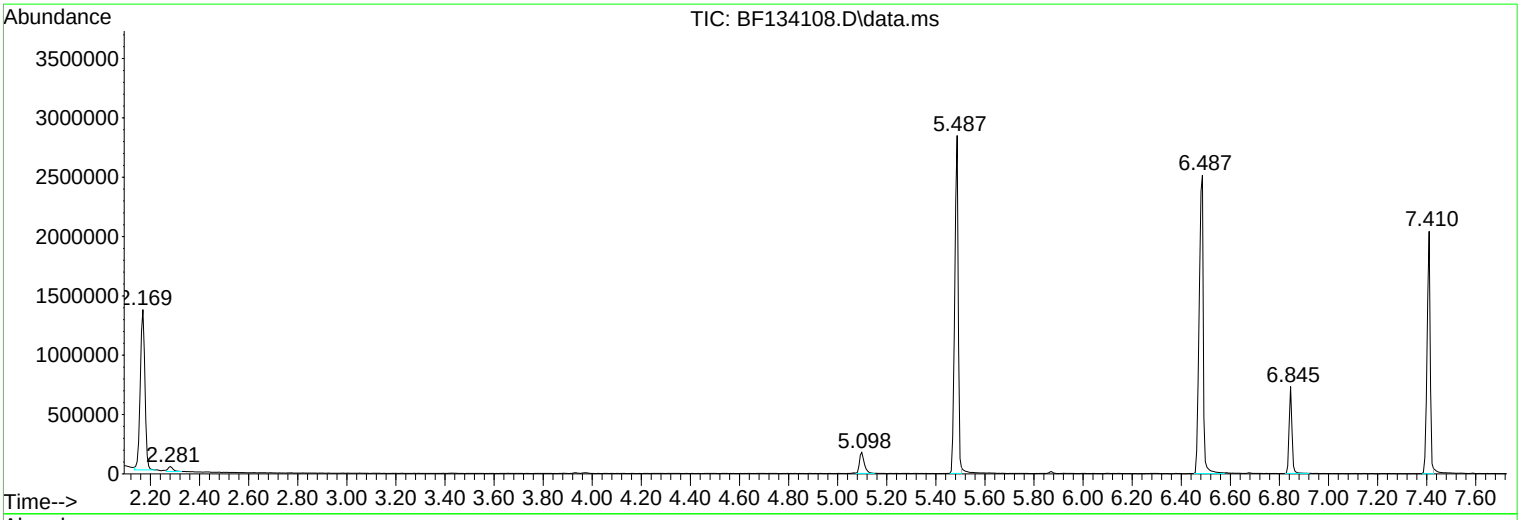
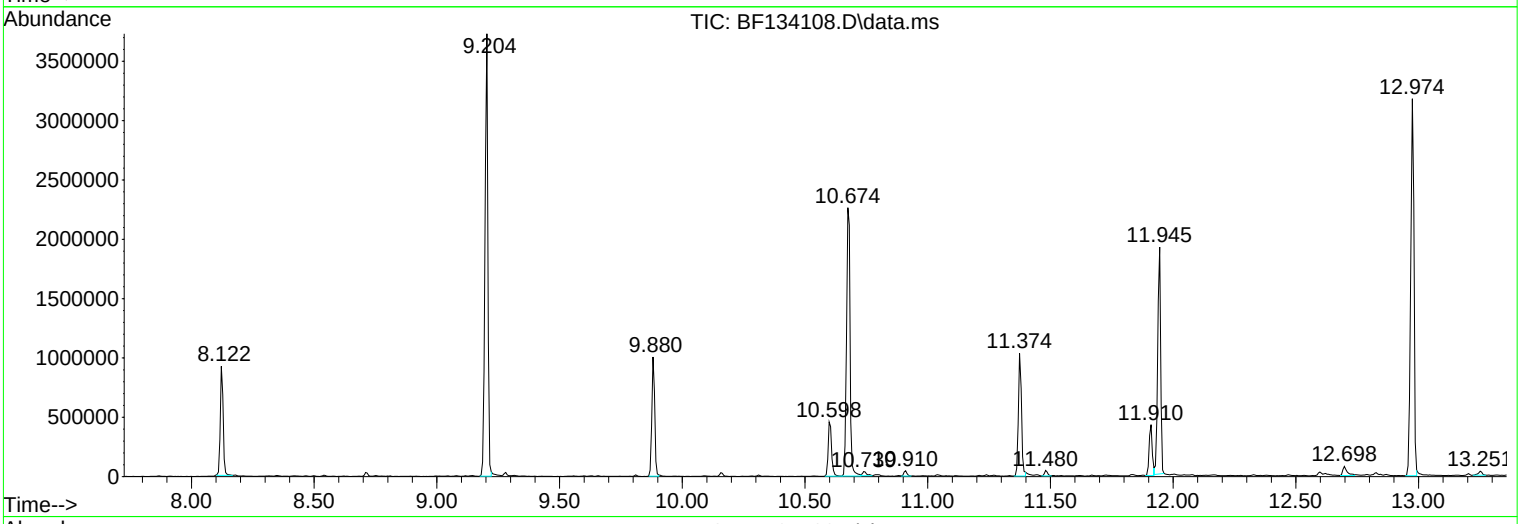
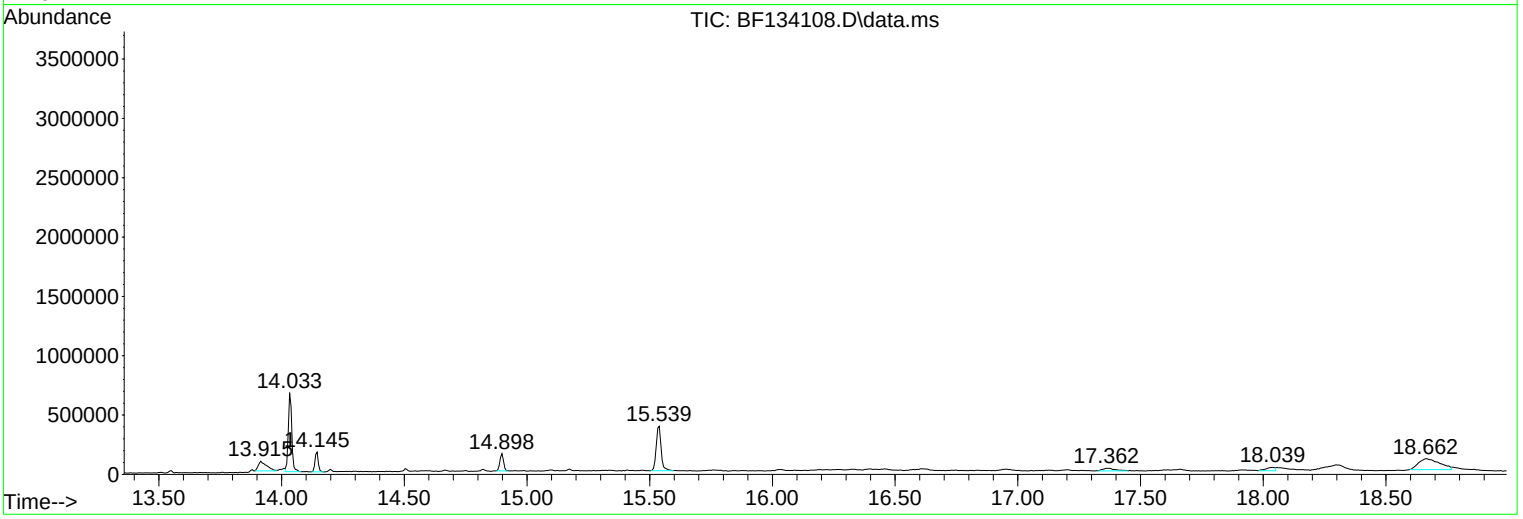
ClientSampleId :
DOREMUS-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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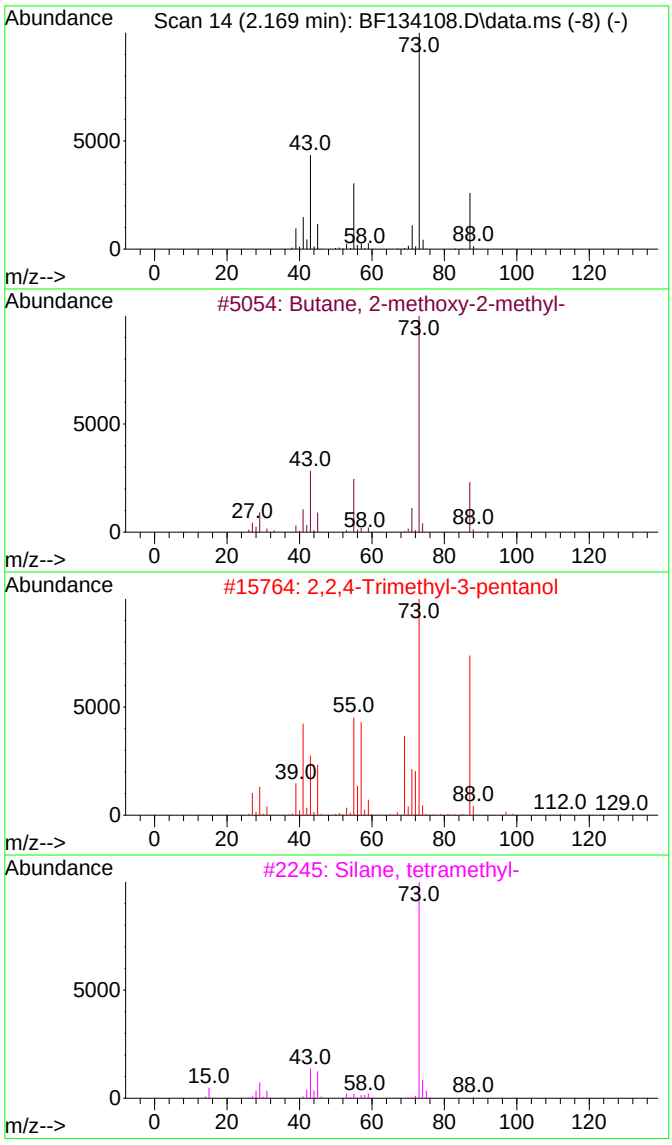
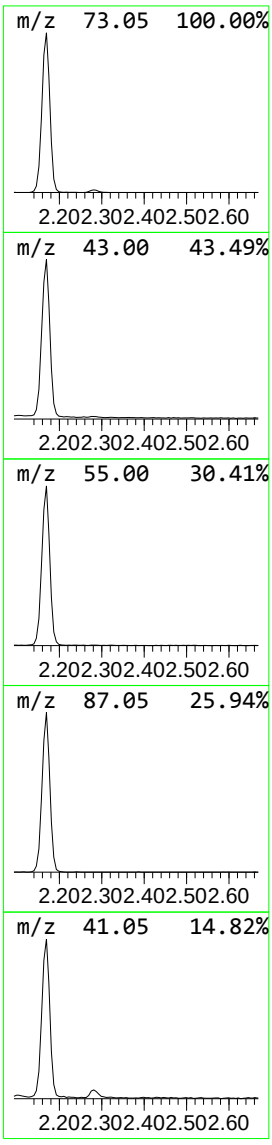
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	60.05 ng	1787200	1,4-Dichlorobenzene-d4	6.845

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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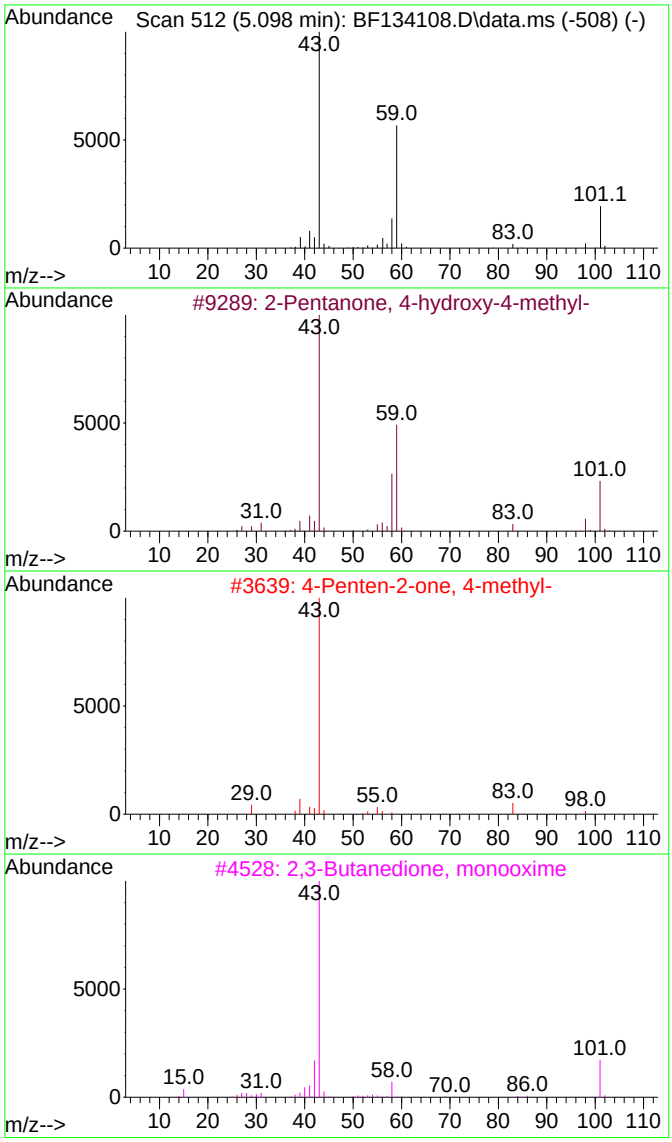
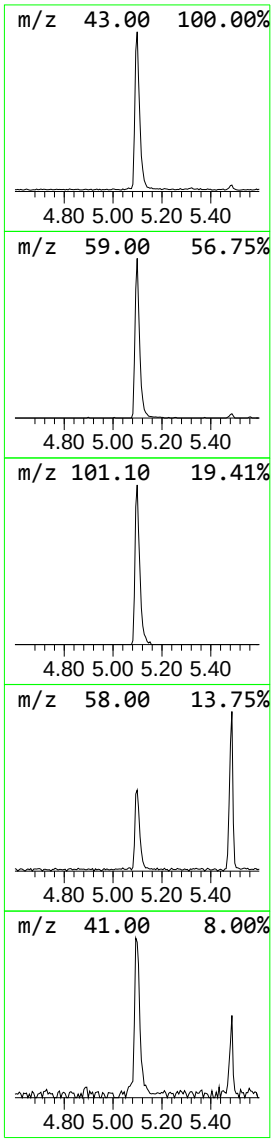
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	8.01 ng	238330	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
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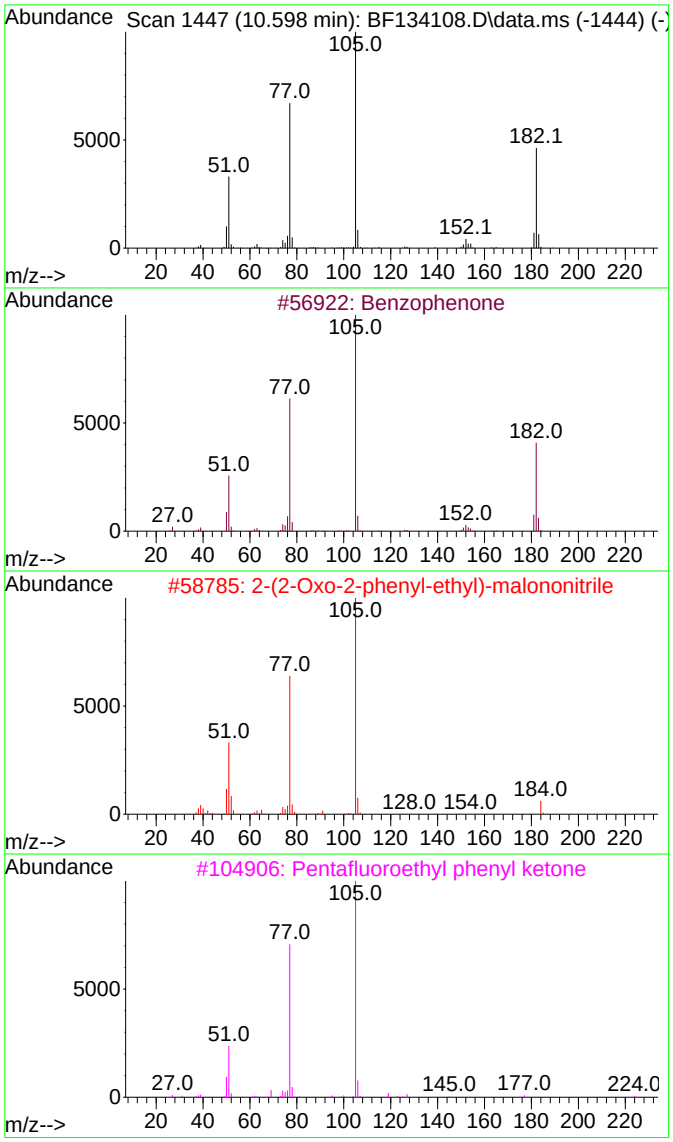
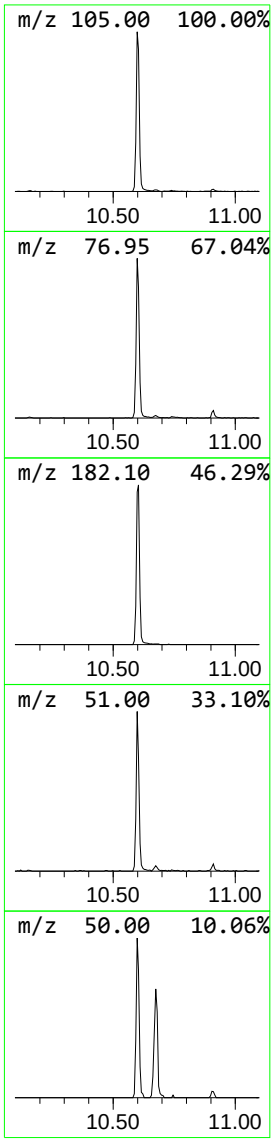
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	10.76 ng	444070	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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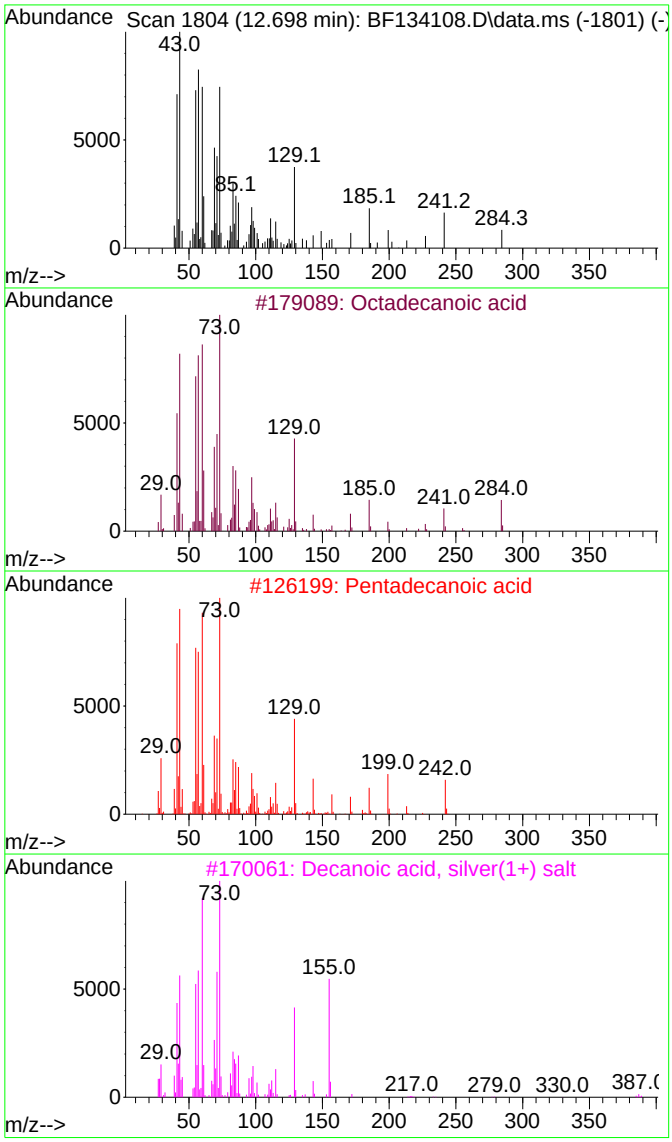
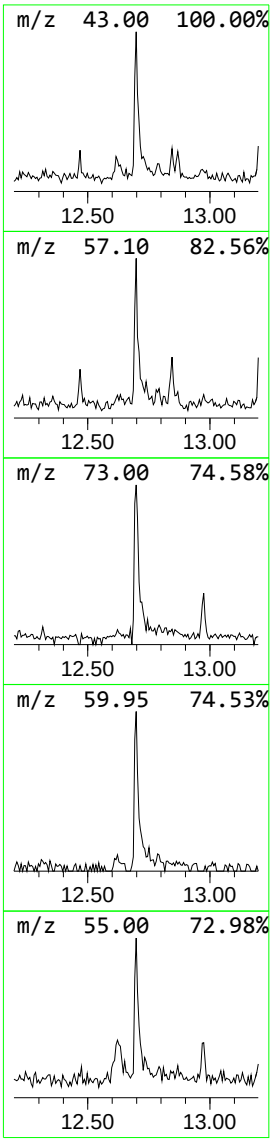
****

Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.15 ng	94951	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	11





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ClientSampleId :
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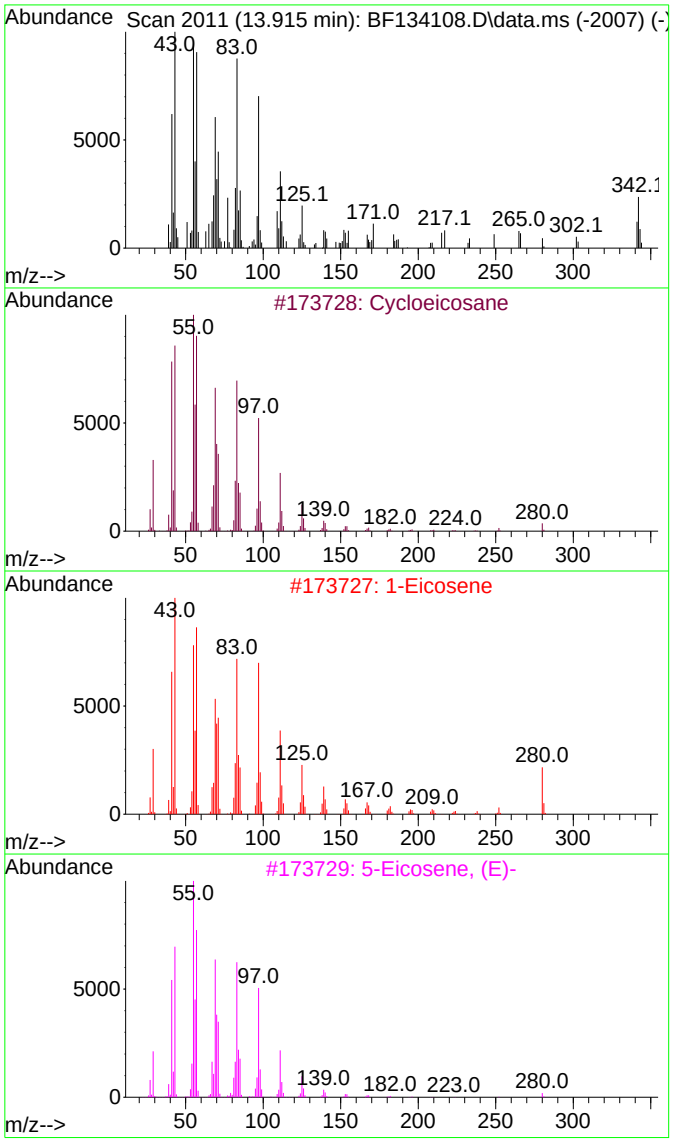
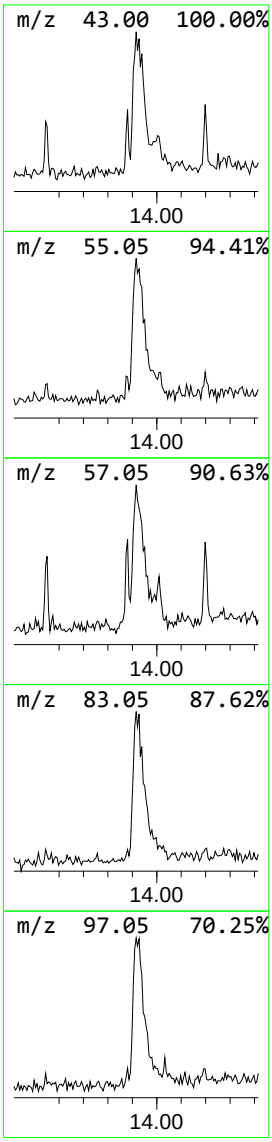
****

Peak Number 5 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	5.81 ng	190046	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	93
2	1-Eicosene	280	C20H40	003452-07-1	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	83





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TIC Library : C:\Database\NIST20.L
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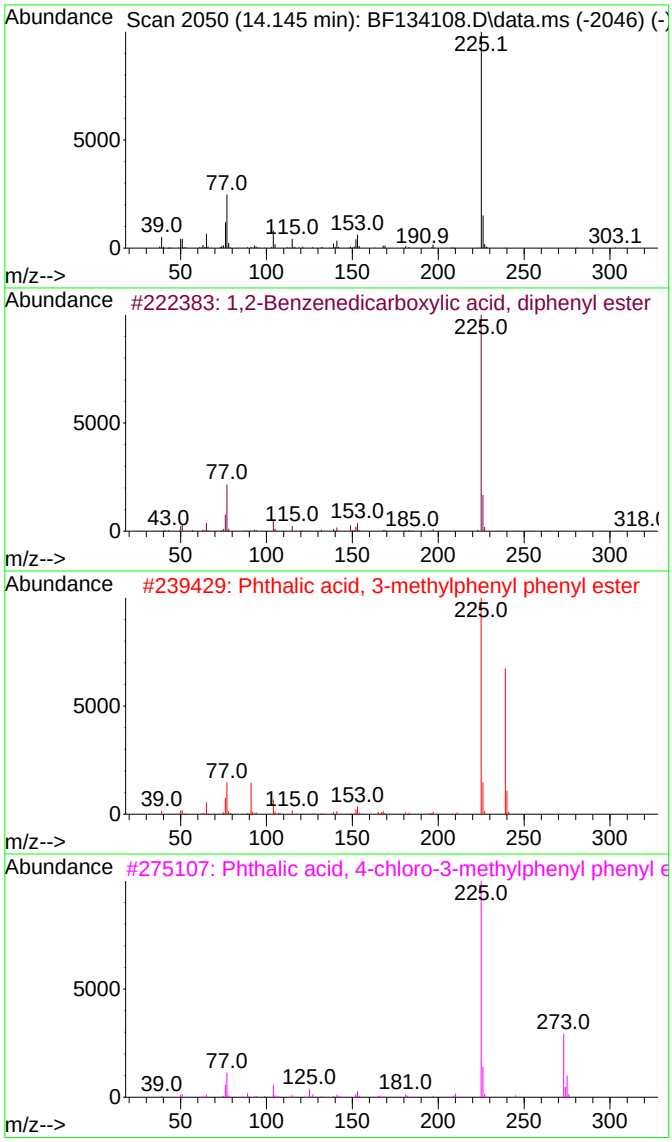
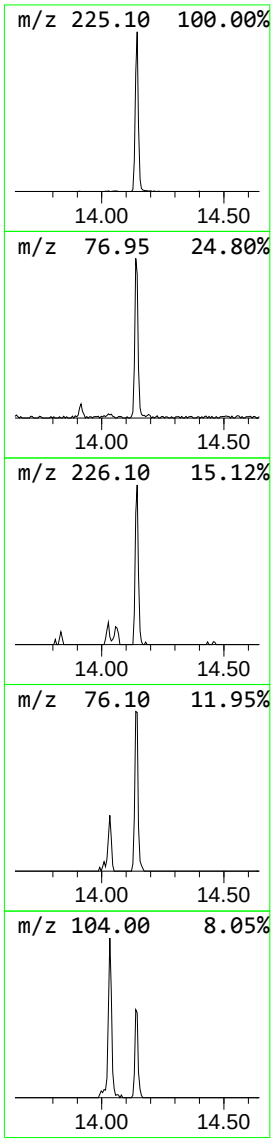
****
Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	4.77 ng	156111	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	318	C20H14O4	000084-62-8	90
2	Phthalic acid, 3-methylphenyl ph...	332	C21H16O4	1000315-60-3	78
3	Phthalic acid, 4-chloro-3-methyl...	366	C21H15ClO4	1000315-71-6	74
4	Phenazine, 1-amino-3-methoxy-	225	C13H11N3O	018450-06-1	72
5	Phthalic acid, 4-isopropylphenyl...	360	C23H20O4	1000315-65-9	72





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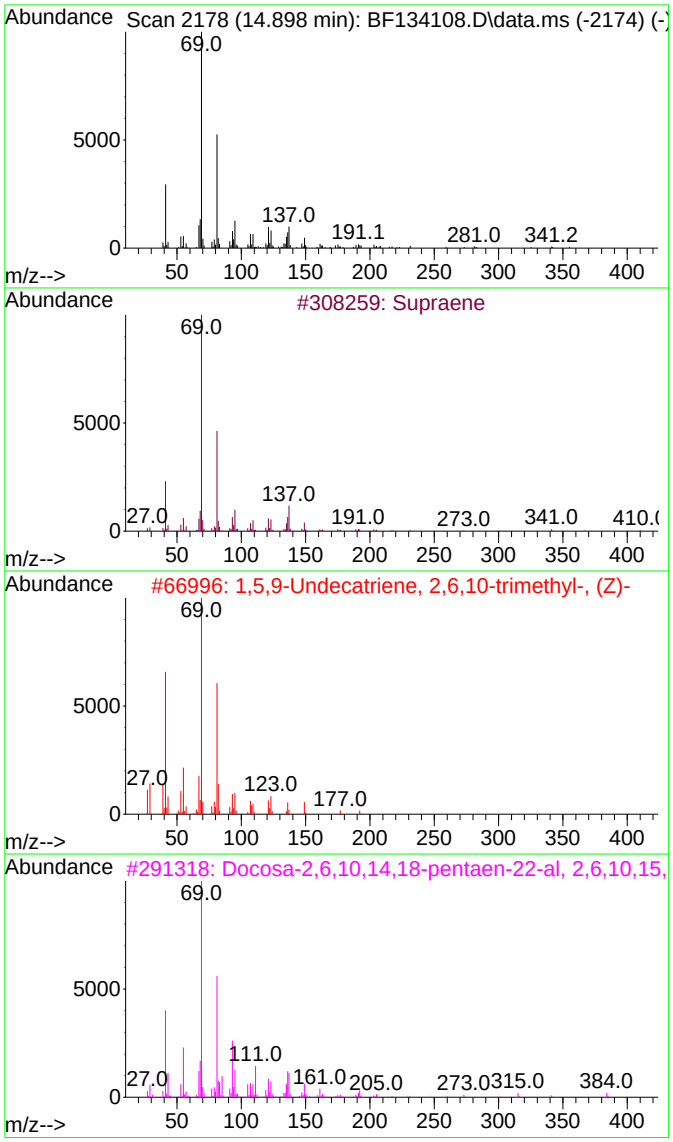
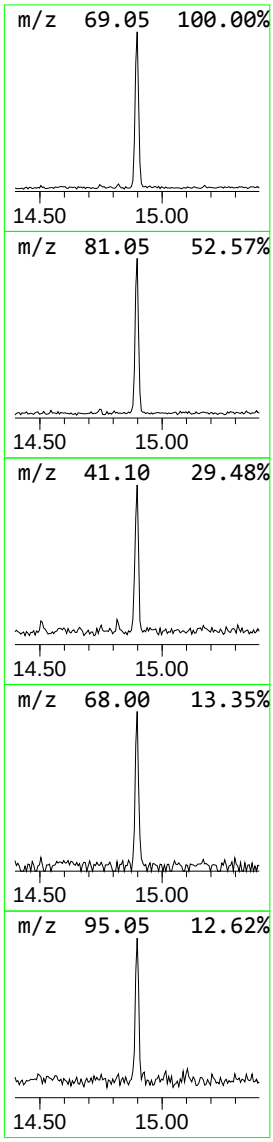
****

Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	5.67 ng	148722	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58





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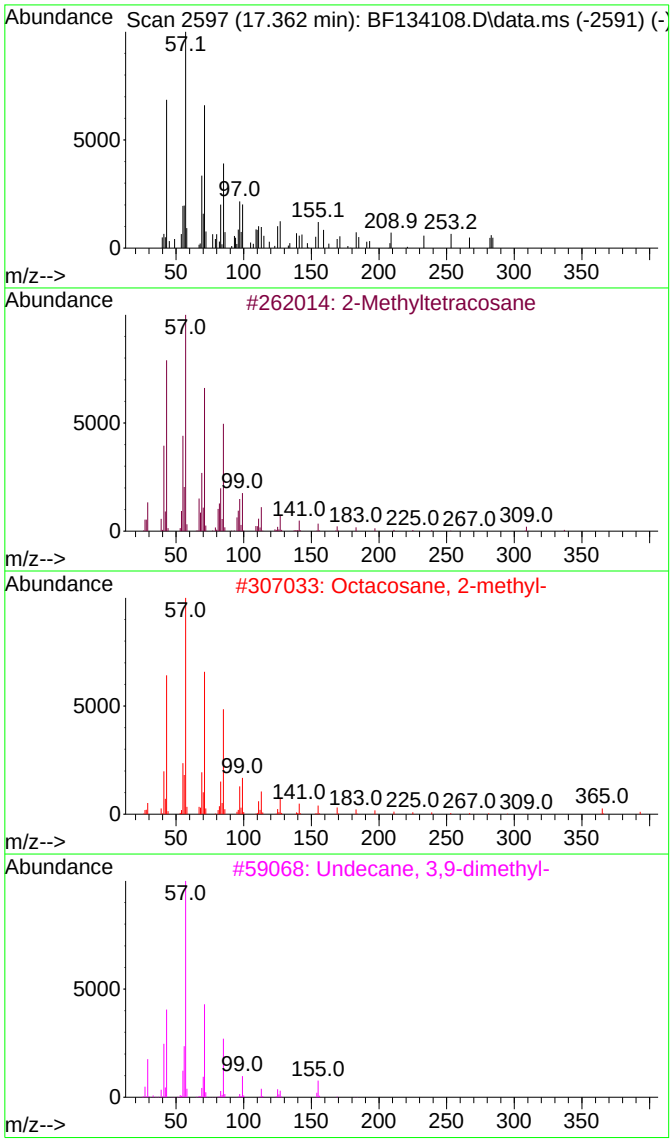
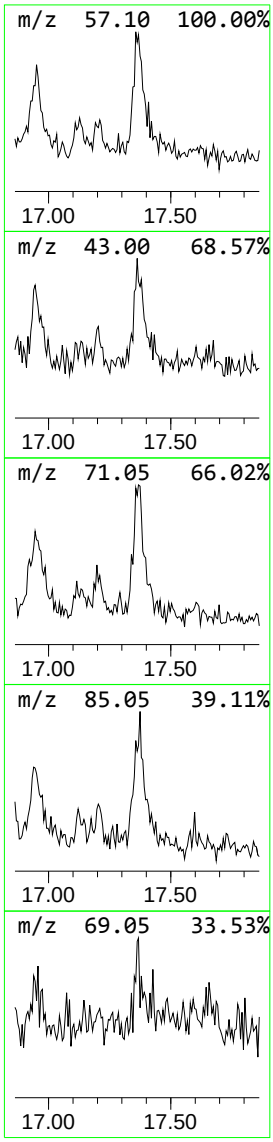
****
Peak Number 8 2-Methyltetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.362	3.04 ng	79853	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyltetracosane	352	C25H52	001560-78-7	64
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	59
3	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	59
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	59
5	Tritetracontane	605	C43H88	007098-21-7	58





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Instrument :
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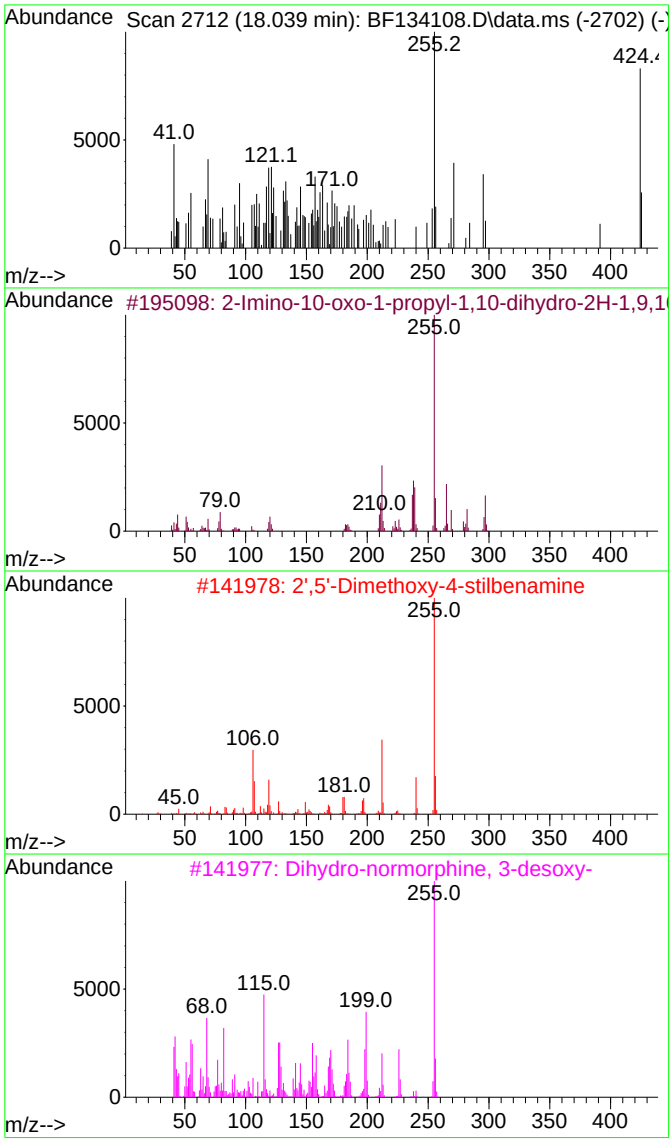
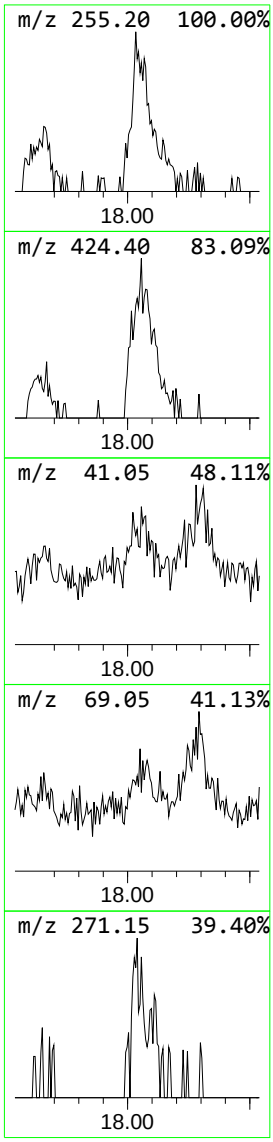
****

Peak Number 9 unknown18.039 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	2.87 ng	75238	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Imino-10-oxo-1-propyl-1,10-dih...	297	C15H15N5O2	1000311-57-3	22
2	2',5'-Dimethoxy-4-stilbenamine	255	C16H17NO2	005803-51-0	18
3	Dihydro-normorphine, 3-desoxy-	255	C16H17NO2	031769-01-4	14
4	N-[2,2,2-Trifluoro-1-(O-toluidin...	342	C14H16F6N2O	1000225-28-3	14
5	Metralindole	255	C15H17N3O	054188-38-4	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134108.D
Acq On : 06 Jul 2023 21:17
Operator : CG\JU
Sample : 03476-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DOREMUS-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

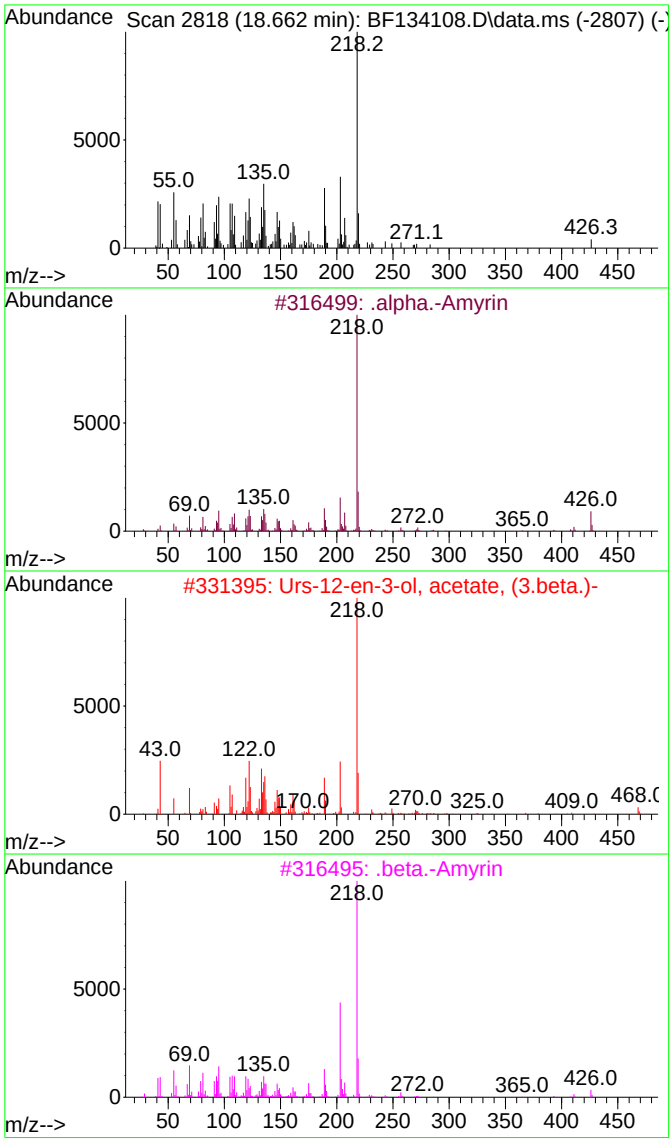
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

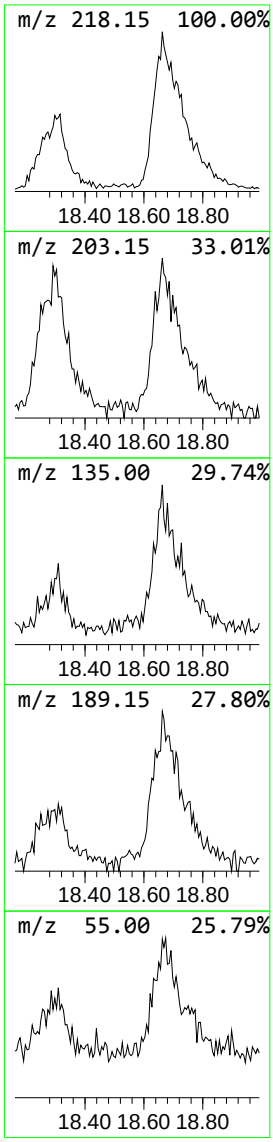
****

Peak Number 10 .alpha.-Amyrin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.662	20.91 ng	548572	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrin	426	C30H50O	000638-95-9	90
2	Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	70
3	.beta.-Amyrin	426	C30H50O	000559-70-6	58
4	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	53
5	p-(3-Methyl-5-oxo-2-pyrazolin-1-...	218	C11H10N2O3	060875-16-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134108.D
Acq On : 06 Jul 2023 21:17
Operator : CG\JU
Sample : 03476-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DOREMUS-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.169	60.0	ng	1787200	1	6.845	595195	20.0
2-Pentanone, 4-...	5.098	8.0	ng	238330	1	6.845	595195	20.0
Benzophenone	10.598	10.8	ng	444070	3	9.880	825215	20.0
Octadecanoic acid	12.698	2.1	ng	94951	4	11.374	883054	20.0
Cycloeicosane	13.916	5.8	ng	190046	5	14.033	654647	20.0
1,2-Benzenedica...	14.145	4.8	ng	156111	5	14.033	654647	20.0
Supraene	14.898	5.7	ng	148722	6	15.539	524721	20.0
2-Methyltetraco...	17.362	3.0	ng	79853	6	15.539	524721	20.0
unknown18.039	18.039	2.9	ng	75238	6	15.539	524721	20.0
.alpha.-Amyrin	18.662	20.9	ng	548572	6	15.539	524721	20.0