LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	17	rBV	1001403	1561133	88.92%	9.241%
2	5.104	508	512	517	rVB	12195	17959	1.02%	0.106%
3	5.498	573	579	585	rBV	1269461	1671025	95.18%	9.891%
4	6.504	744	750	755	rBV	1246901	1647874	93.86%	9.754%
5	6.539	755	756	768	rVB4	10686	18255	1.04%	0.108%
6	6.716	782	786	791	rBV2	13156	19145	1.09%	0.113%
7	6.887	810	815	821	rVB	497407	615932	35.08%	3.646%
8	7.445	901	910	915	rBV	870209	1098701	62.58%	6.504%
9	7.698	946	953	960	rVB3	19520	31271	1.78%	0.185%
10	8.169	1026	1033	1040	rBV	595795	766065	43.63%	4.535%
11	8.463	1076	1083	1089	rBV10	10041	18060	1.03%	0.107%
12	8.586	1101	1104	1110	rBV	14849	21810	1.24%	0.129%
13	8.757	1129	1133	1137	rBV	31714	37567	2.14%	0.222%
14	8.881	1150	1154	1158	rVB	25005	30409	1.73%	0.180%
15	9.186	1203	1206	1210	rVB	15939	19349	1.10%	0.115%
16	9.245	1210	1216	1225	rBV	1329814	1755691	100.00%	10.393%
17	9.322	1225	1229	1234	rVB	44234	59134	3.37%	0.350%
18	9.504	1256	1260	1265	rBV	18045	26663	1.52%	0.158%
19	9.580	1269	1273	1275	rBV	27438	34277	1.95%	0.203%
20	9.639	1280	1283	1290	rVB3	28543	44008	2.51%	0.260%
21	9.698	1290	1293	1304	rVB3	12508	24415	1.39%	0.145%
22	9.851	1312	1319	1324	rBV	37670	56996	3.25%	0.337%
23	9.922	1324	1331	1336	rBV	536223	675831	38.49%	4.000%
24	10.122	1361	1365	1369	rVB3	12818	17719	1.01%	0.105%
25	10.169	1369	1373	1379	rVB4	12389	18273	1.04%	0.108%
26	10.351	1396	1404	1408	rBV2	47723	69680	3.97%	0.412%
27	10.575	1436	1442	1447	rBV	24813	41889	2.39%	0.248%
28	10.633	1447	1452	1459	rVV	243596	311493	17.74%	1.844%
29	10.710	1459	1465	1478	rVV	625740	832048	47.39%	4.925%
30	10.827	1480	1485	1494	rVB	77468	133591	7.61%	0.791%
31	10.945	1501	1505	1509	rVB	25730	27960	1.59%	0.166%
32	11.274	1556	1561	1564	rBV	66564	91586	5.22%	0.542%
33	11.304	1564	1566	1572	rVB	33019	39902	2.27%	0.236%
34	11.410	1579	1584	1592	rBV2	474950	686099	39.08%	4.061%
35	11.480	1592	1596	1600	rVB2	25512	38398	2.19%	0.227%
36	11.698	1629	1633	1638	rBV	57473	70116	3.99%	0.415%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.933	1666	1673	1682	rBV2	176168	285623	16.27%	1.691%
38	12.021	1686	1688	1696	rVB4	22593	38326	2.18%	0.227%
39	12.110	1698	1703	1707	rBV	57429	74449	4.24%	0.441%
40	12.498	1765	1769	1775	rBV	51996	64750	3.69%	0.383%
41	12.621	1785	1790	1796	rBV	111556	153958	8.77%	0.911%
42	12.716	1802	1806	1813	rBV	45160	84320	4.80%	0.499%
43	12.851	1824	1829	1836	rBV2	87985	173858	9.90%	1.029%
44	12.992	1848	1853	1862	rBV	1209871	1588175	90.46%	9.401%
45	13.227	1889	1893	1899	rBV2	38665	82759	4.71%	0.490%
46	13.568	1947	1951	1957	rBV2	40879	71883	4.09%	0.426%
47	13.898	2003	2007	2016	rVB	86074	164922	9.39%	0.976%
48	14.051	2027	2033	2043	rVB	490423	750565	42.75%	4.443%
49	14.810	2159	2162	2174	rVB2	69198	144138	8.21%	0.853%
50	15.527	2279	2284	2296	rVB	337659	585656	33.36%	3.467%

Sum of corrected areas: 16893706

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
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Operator : RC/JU
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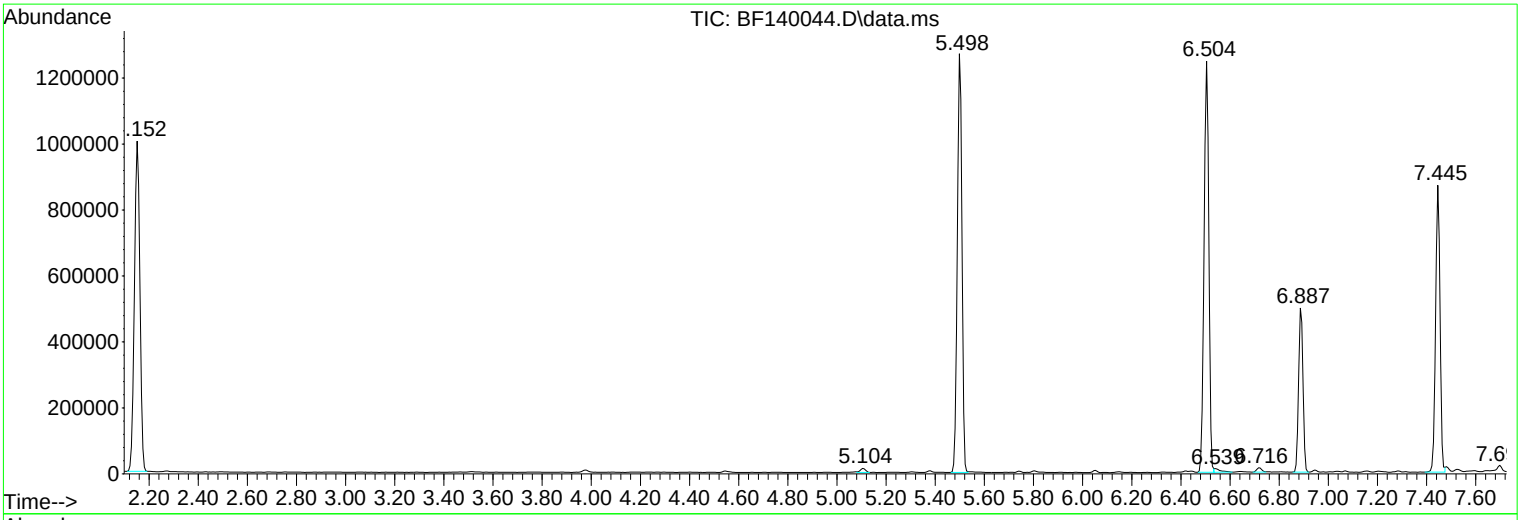
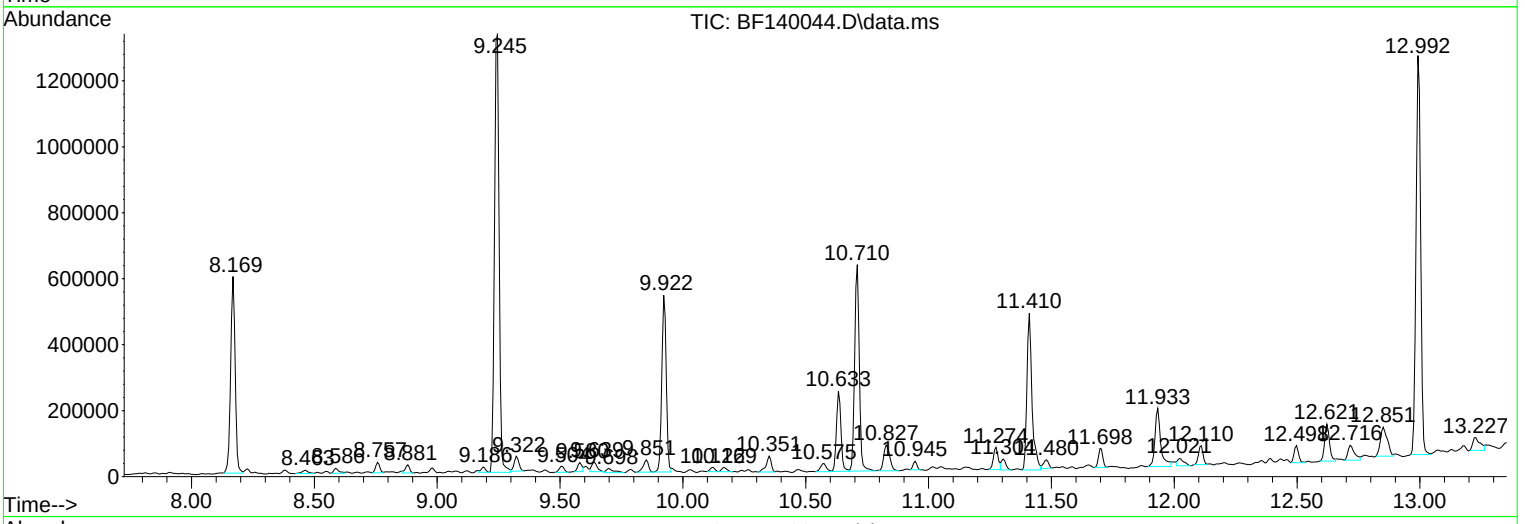
Misc :
ALS Vial : 20 Sample Multiplier: 1

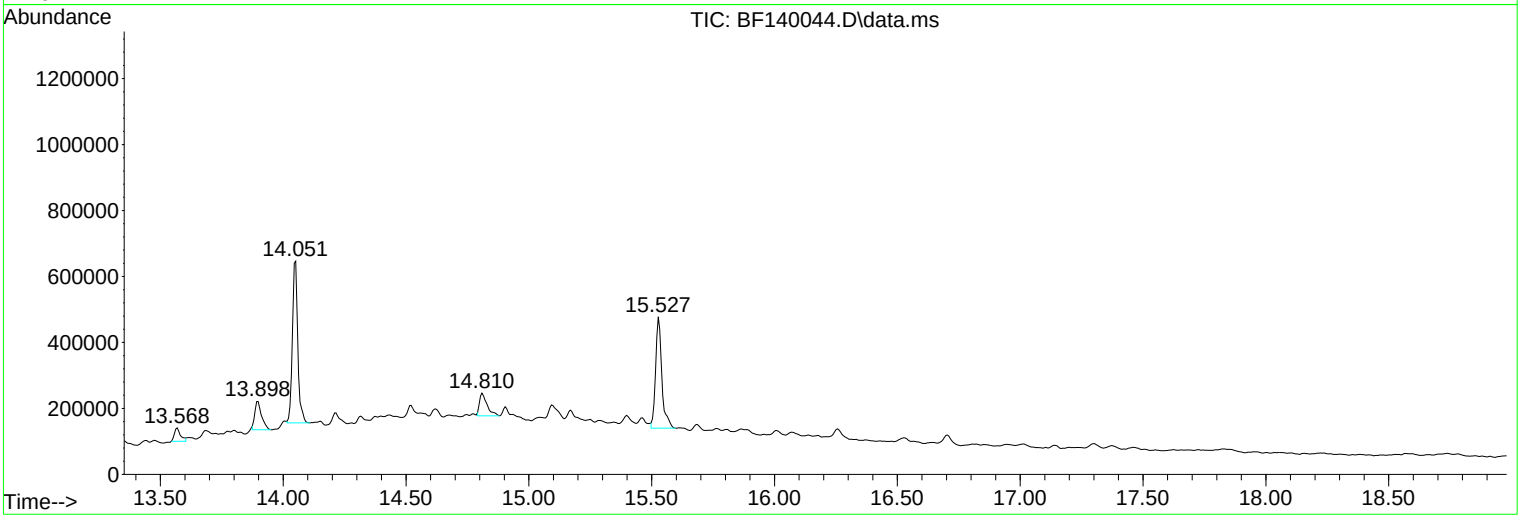
Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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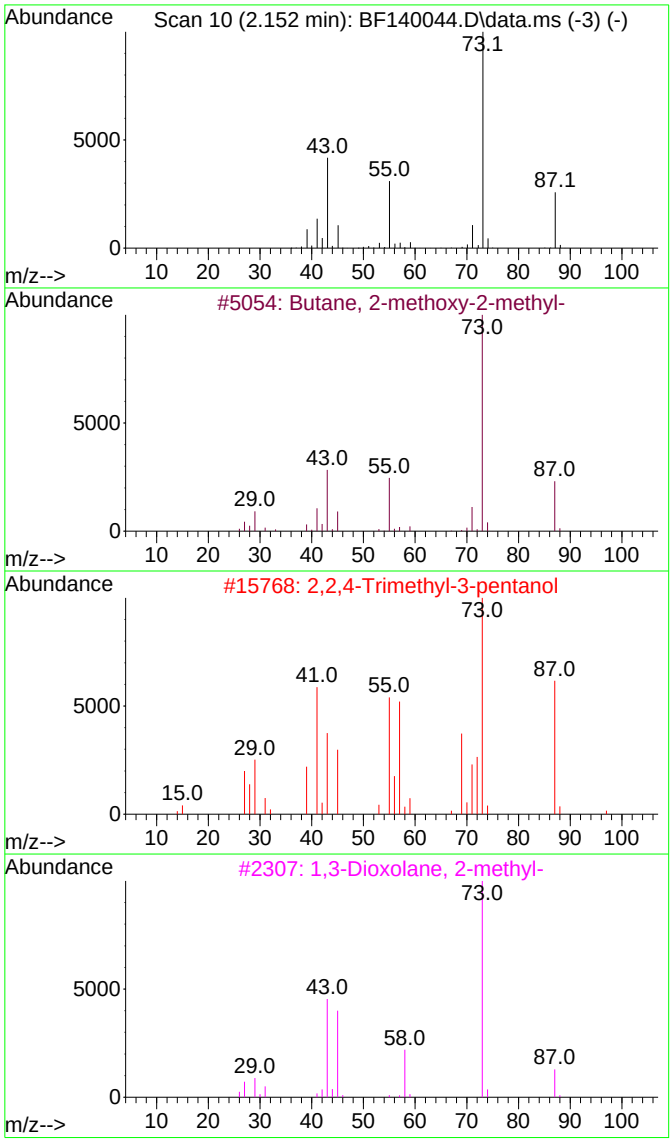
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

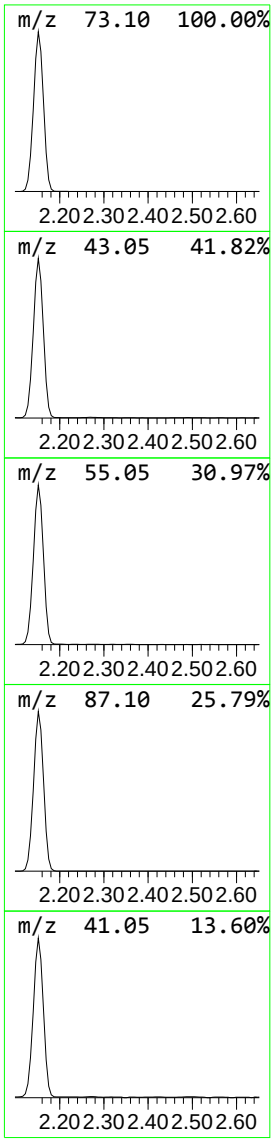
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	50.69 ng	1561130	1,4-Dichlorobenzene-d4	6.887

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

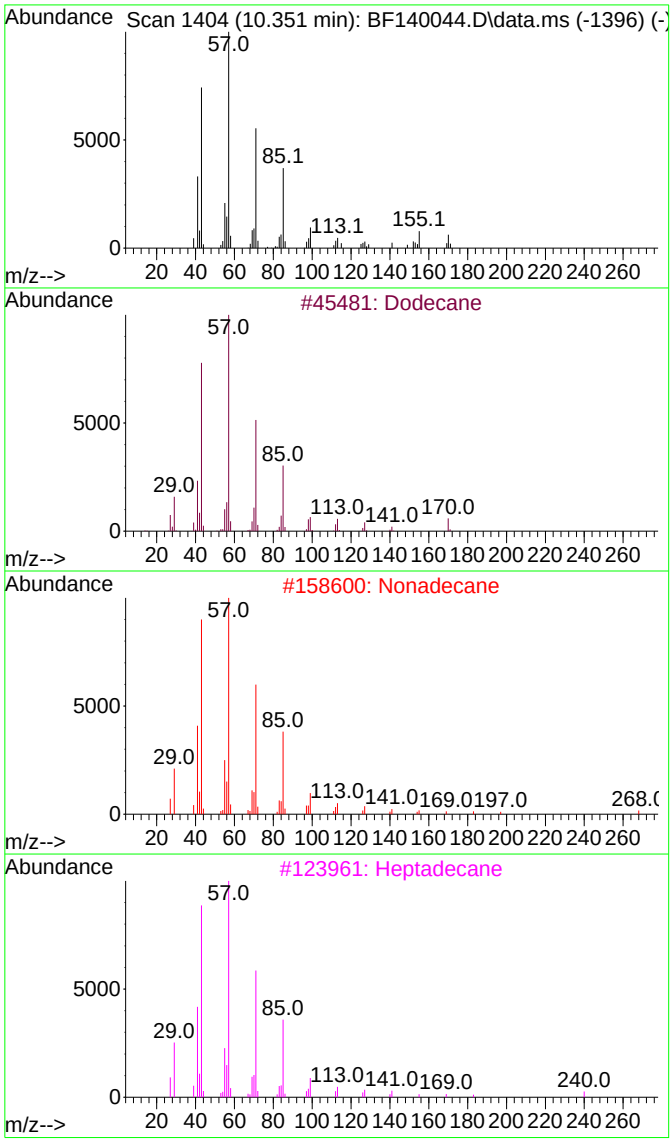
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

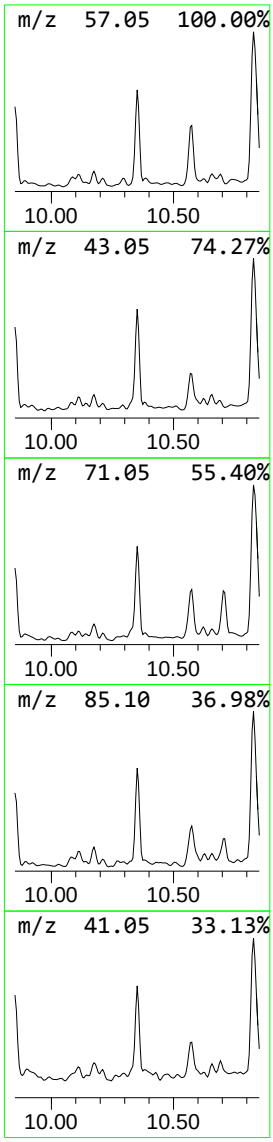
****

Peak Number 2 Dodecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.351	2.06 ng	69680	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	94
2	Nonadecane	268	C19H40	000629-92-5	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tridecane	184	C13H28	000629-50-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

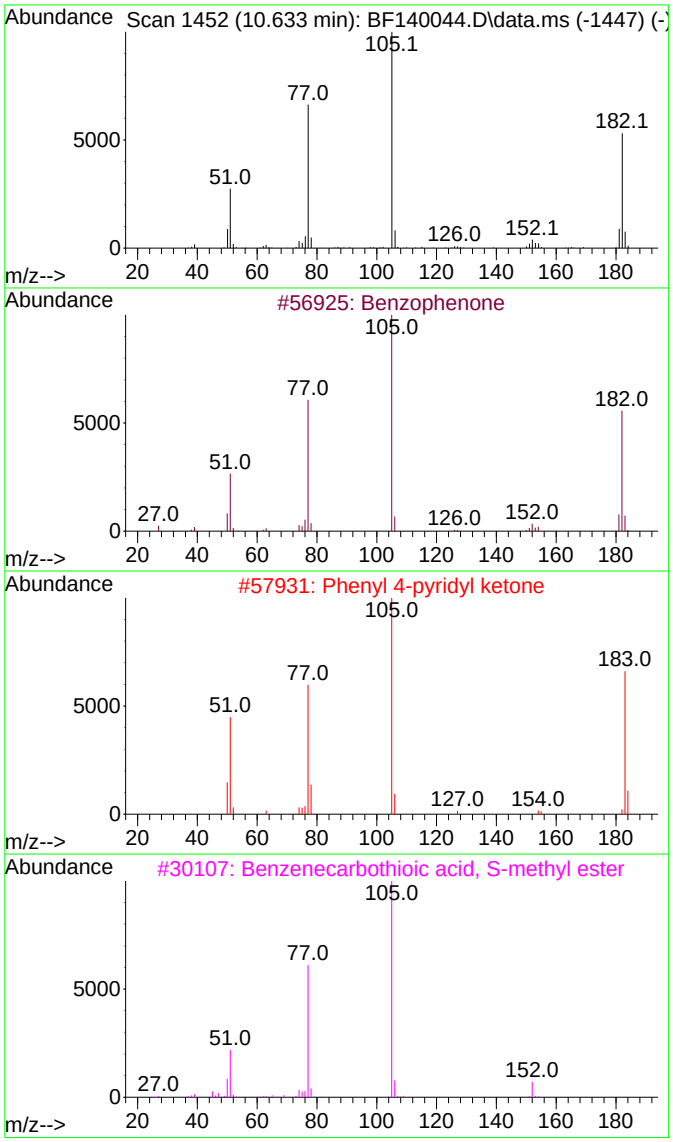
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

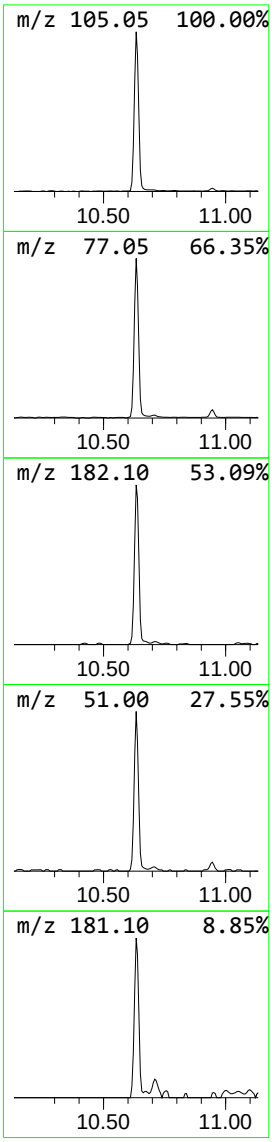
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	9.22 ng	311493	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

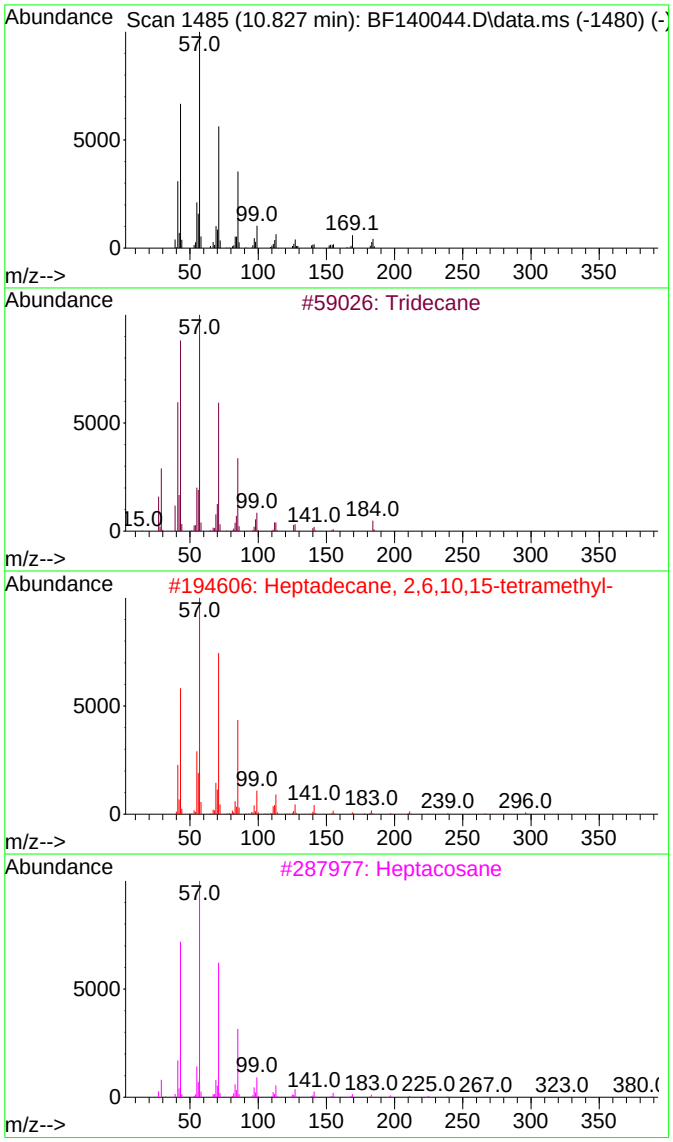
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

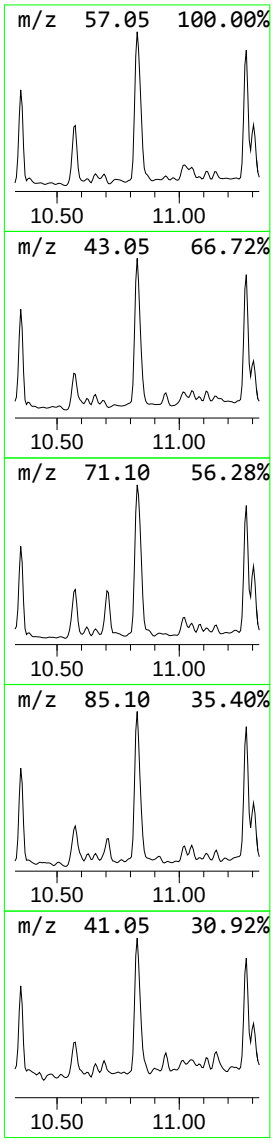
****

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	3.89 ng	133591	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
5	Nonadecane	268	C19H40	000629-92-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

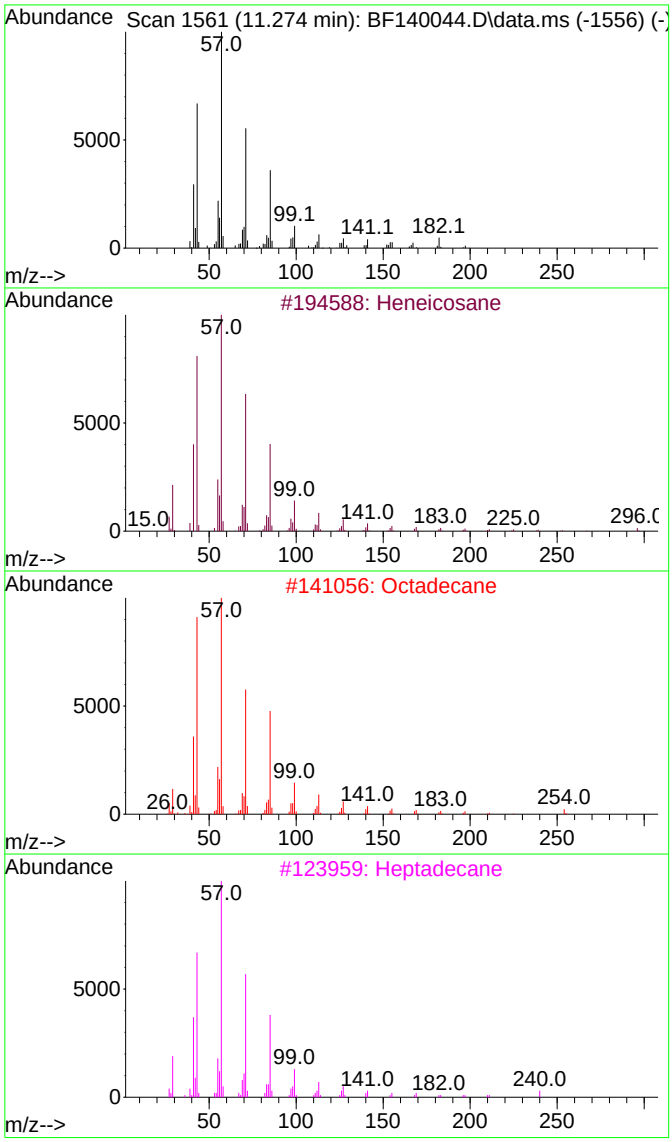
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

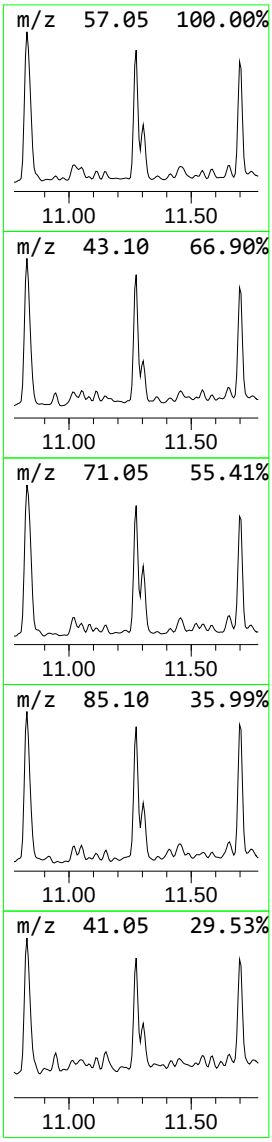
****

Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	2.67 ng	91586	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Nonadecane	268	C19H40	000629-92-5	90
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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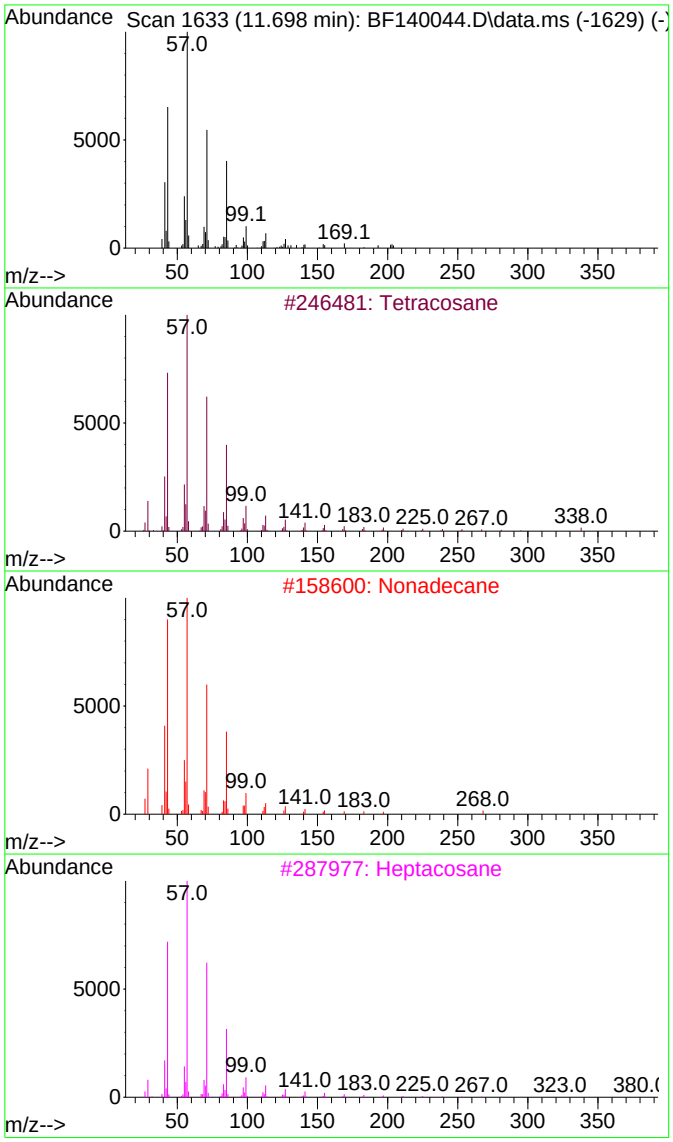
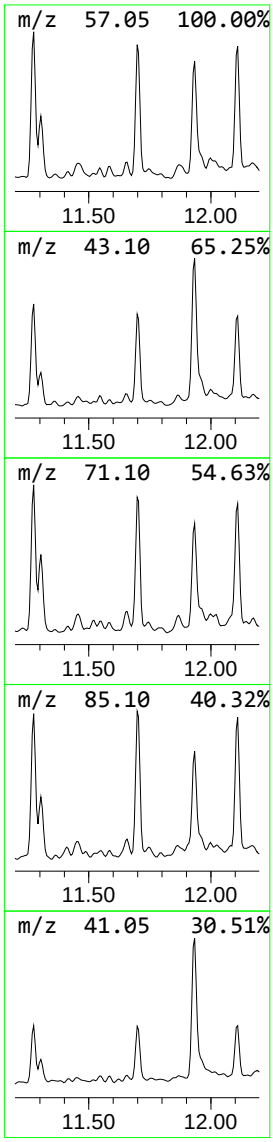
Peak Number 6 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	2.04 ng	70116	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Nonadecane	268	C19H40	000629-92-5	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Octadecane	254	C18H38	000593-45-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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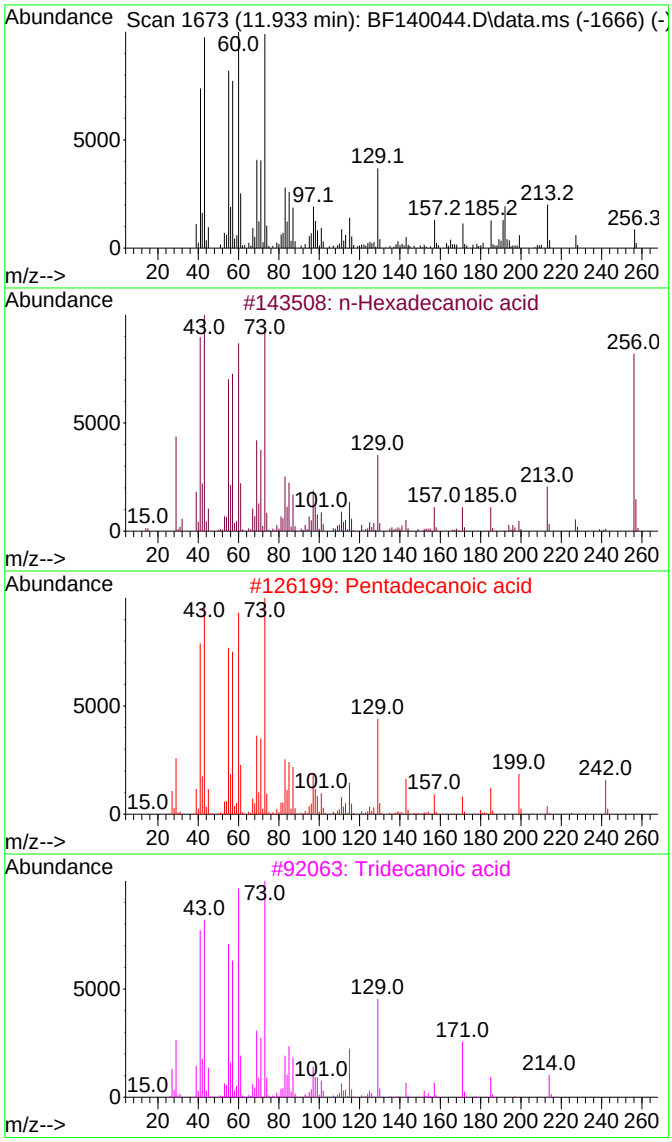
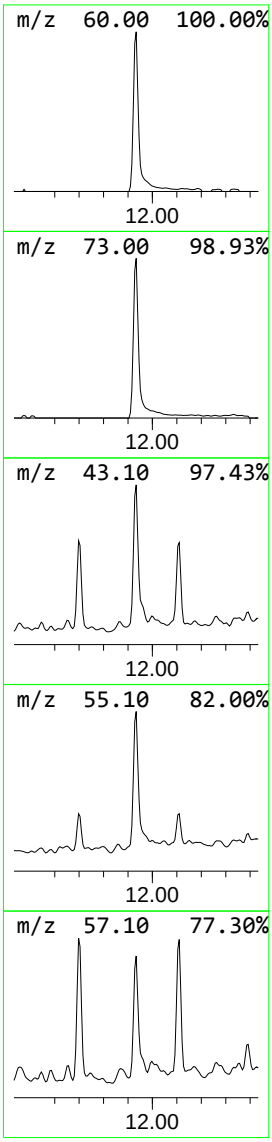
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	8.33 ng	285623	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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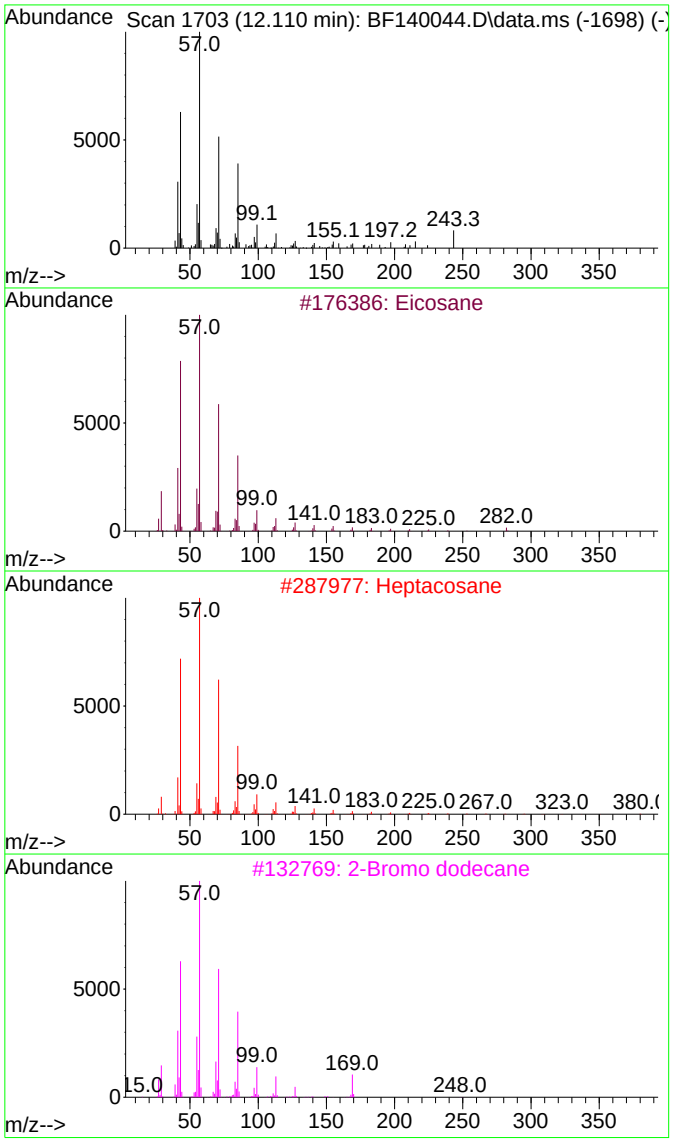
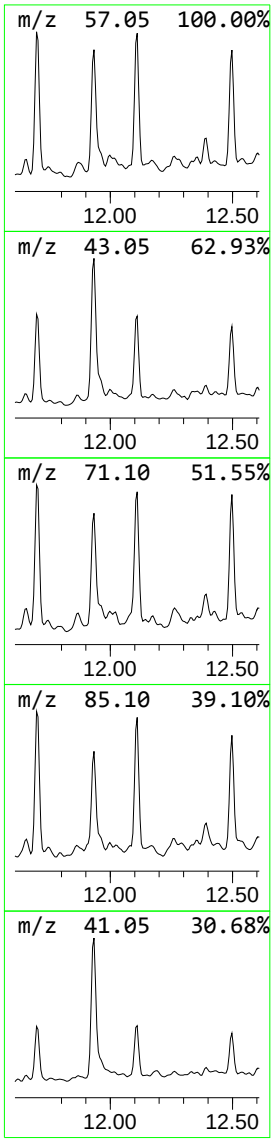
Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.17 ng	74449	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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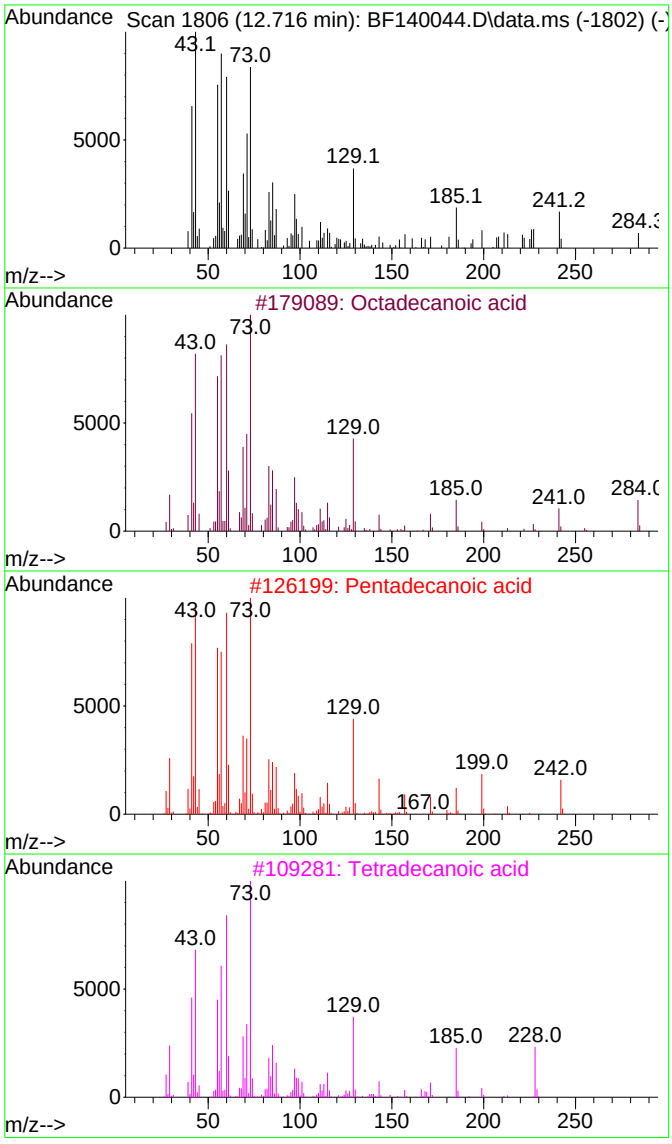
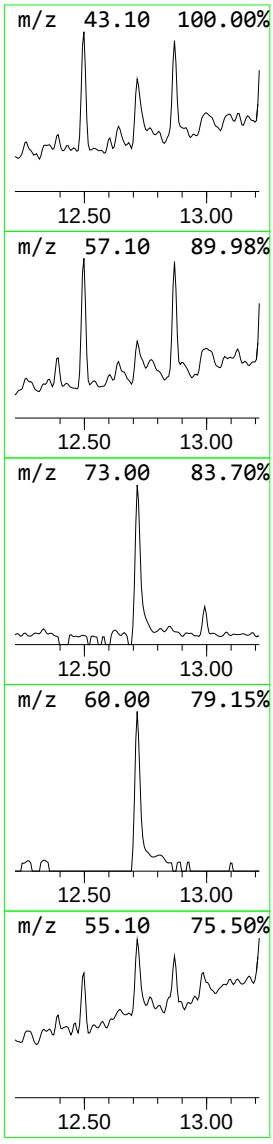
Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.46 ng	84320	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Hexadecane	226	C16H34	000544-76-3	25





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Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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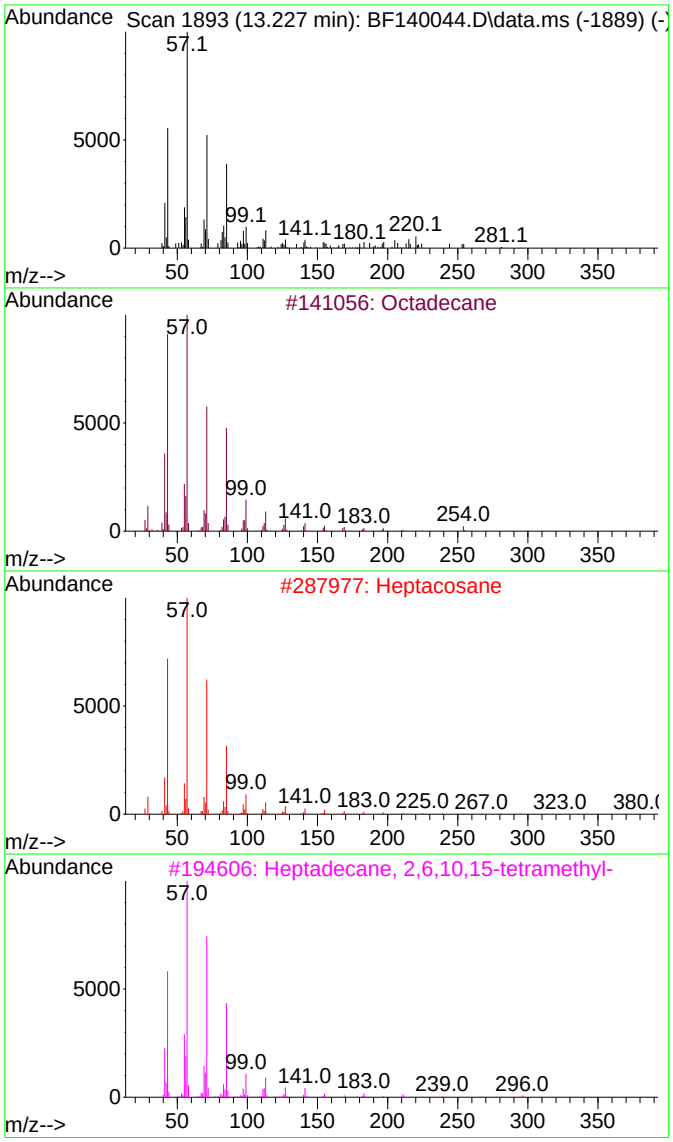
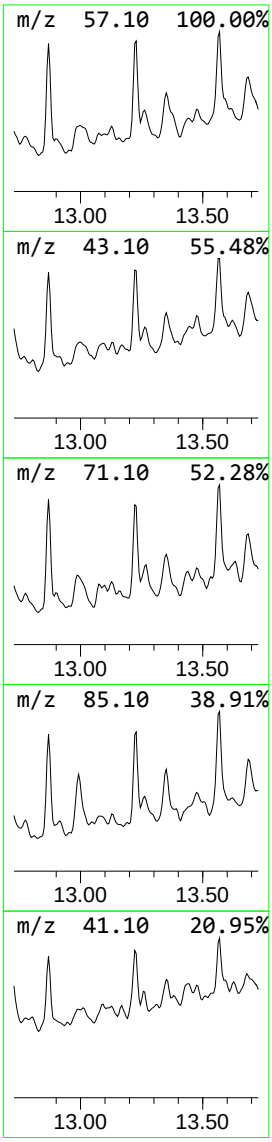
Peak Number 10 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	2.21 ng	82759	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Heptacosane	380	C27H56	000593-49-7	83
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Heptadecane	240	C17H36	000629-78-7	80





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Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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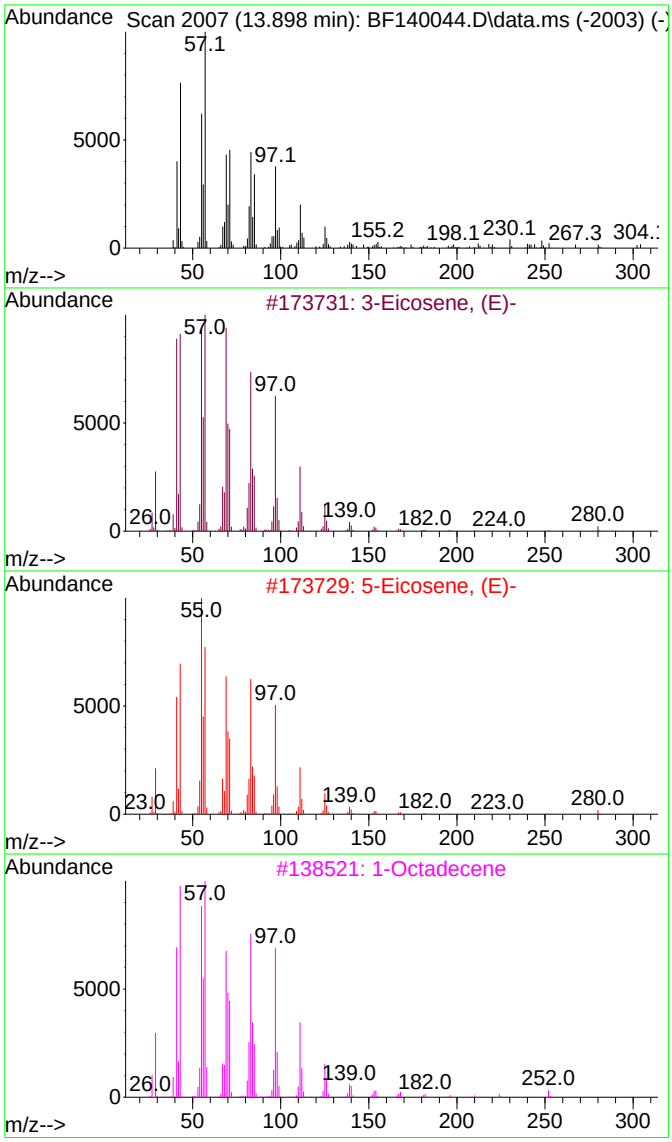
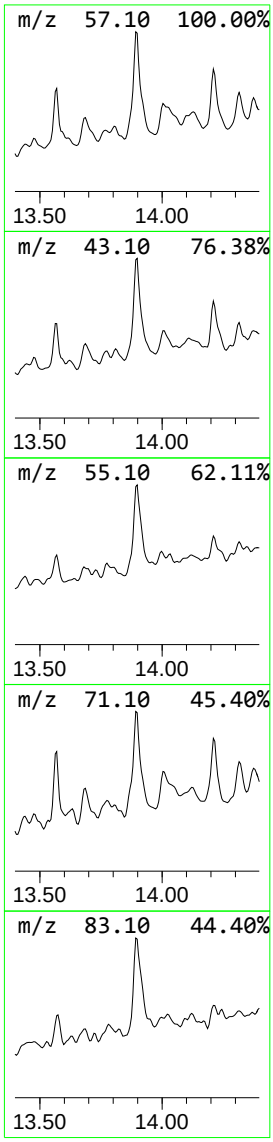
Peak Number 11 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.39 ng	164922	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	1-Octadecene	252	C18H36	000112-88-9	93
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91





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Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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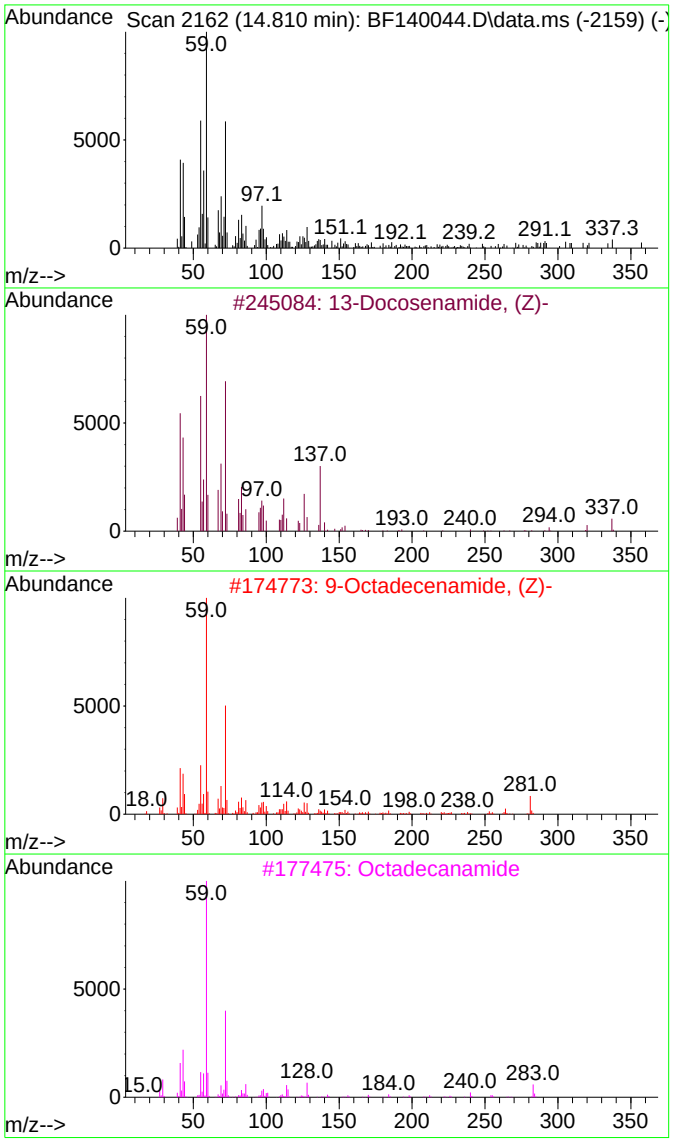
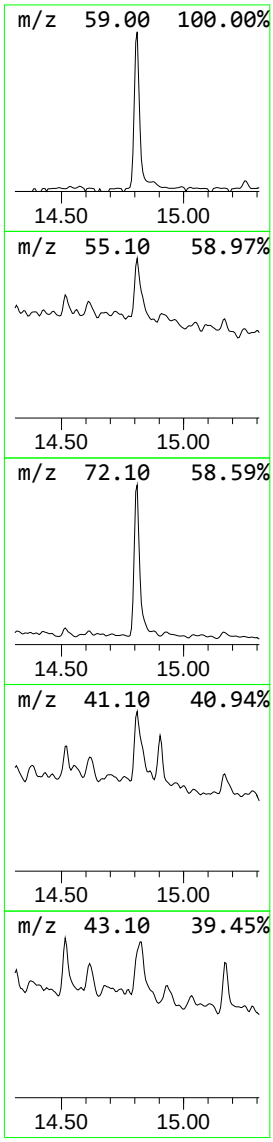
Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	4.92 ng	144138	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
3	Octadecanamide	283	C18H37NO	000124-26-5	64
4	Silane, hexyl-	116	C6H16Si	001072-14-6	46
5	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140044.D
Acq On : 25 Oct 2024 18:21
Operator : RC/JU
Sample : P4472-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.152	50.7	ng	1561130	1	6.887	615932	20.0
Dodecane	10.351	2.1	ng	69680	3	9.922	675831	20.0
Benzophenone	10.633	9.2	ng	311493	3	9.922	675831	20.0
Tridecane	10.828	3.9	ng	133591	4	11.410	686099	20.0
Heneicosane	11.275	2.7	ng	91586	4	11.410	686099	20.0
Tetracosane	11.698	2.0	ng	70116	4	11.410	686099	20.0
n-Hexadecanoic ...	11.933	8.3	ng	285623	4	11.410	686099	20.0
Eicosane	12.110	2.2	ng	74449	4	11.410	686099	20.0
Octadecanoic acid	12.716	2.5	ng	84320	4	11.410	686099	20.0
Octadecane	13.227	2.2	ng	82759	5	14.051	750565	20.0
3-Eicosene, (E)-	13.898	4.4	ng	164922	5	14.051	750565	20.0
13-Docosenamide...	14.810	4.9	ng	144138	6	15.527	585656	20.0