LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133107.D
Acq On : 27 Apr 2023 18:55
Operator : CG\JU
Sample : 02503-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-305A-COMP-03

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.452	59	62	70	rVB	40267	60337	1.00%	0.126%
2	4.940	481	485	493	rVB	67078	84452	1.40%	0.176%
3	5.346	549	554	558	rBV	3975658	4293077	71.32%	8.961%
4	6.375	723	729	732	rBV	4254784	4544589	75.50%	9.486%
5	6.734	786	790	793	rBV	1517800	1170976	19.45%	2.444%
6	7.298	880	886	889	rBV	2976853	2754883	45.76%	5.750%
7	8.016	1003	1008	1011	rBV	2035382	1631963	27.11%	3.406%
8	9.098	1186	1192	1195	rBV	5184388	4918132	81.70%	10.265%
9	9.769	1302	1306	1309	rBV	2473855	1874229	31.14%	3.912%
10	9.986	1338	1343	1353	rBV	498415	447362	7.43%	0.934%
11	10.480	1424	1427	1431	rBV	567256	433101	7.19%	0.904%
12	10.557	1435	1440	1443	rBV	3603068	3282722	54.53%	6.852%
13	10.786	1476	1479	1483	rVB	124762	93349	1.55%	0.195%
14	10.875	1490	1494	1498	rBV	139956	148411	2.47%	0.310%
15	10.928	1498	1503	1509	rBV	607427	568405	9.44%	1.186%
16	11.169	1541	1544	1548	rVB	81957	62858	1.04%	0.131%
17	11.251	1554	1558	1561	rBV	2263219	1891116	31.42%	3.947%
18	11.322	1566	1570	1573	rVB2	82485	72154	1.20%	0.151%
19	11.716	1632	1637	1641	rBV	267078	282072	4.69%	0.589%
20	11.798	1646	1651	1659	rVV	2085291	2201046	36.56%	4.594%
21	12.457	1760	1763	1764	rBV	81786	65211	1.08%	0.136%
22	12.510	1764	1772	1781	rVV	3831272	6019639	100.00%	12.565%
23	12.580	1781	1784	1797	rVV	932508	1061374	17.63%	2.215%
24	12.686	1797	1802	1805	rVB	67723	83502	1.39%	0.174%
25	12.839	1823	1828	1831	rBV	5040939	4882551	81.11%	10.191%
26	13.080	1865	1869	1872	rBV	360825	308144	5.12%	0.643%
27	13.327	1908	1911	1918	rVB	102021	99310	1.65%	0.207%
28	13.421	1923	1927	1929	rBV	113898	90643	1.51%	0.189%
29	13.680	1965	1971	1976	rBV2	137819	152757	2.54%	0.319%
30	13.751	1979	1983	1986	rVV	659092	597921	9.93%	1.248%
31	13.851	1991	2000	2002	rBV3	154440	309065	5.13%	0.645%
32	13.880	2002	2005	2008	rVB	1495496	1315704	21.86%	2.746%
33	13.980	2018	2022	2032	rVB	252786	280166	4.65%	0.585%
34	14.063	2033	2036	2042	rVB	90242	88540	1.47%	0.185%
35	14.368	2084	2088	2091	rBV	246767	208271	3.46%	0.435%
36	14.992	2190	2194	2198	rVB	68072	75247	1.25%	0.157%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-03

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.304	2241	2247	2252	rBV	954234	1130021	18.77%	2.359%
38	15.762	2321	2325	2331	rBV2	40484	61206	1.02%	0.128%
39	16.245	2401	2407	2409	rBV3	65802	122283	2.03%	0.255%
40	16.798	2496	2501	2507	rVB3	33896	60870	1.01%	0.127%
41	17.451	2607	2612	2621	rBV4	34295	81770	1.36%	0.171%

Sum of corrected areas: 47909429

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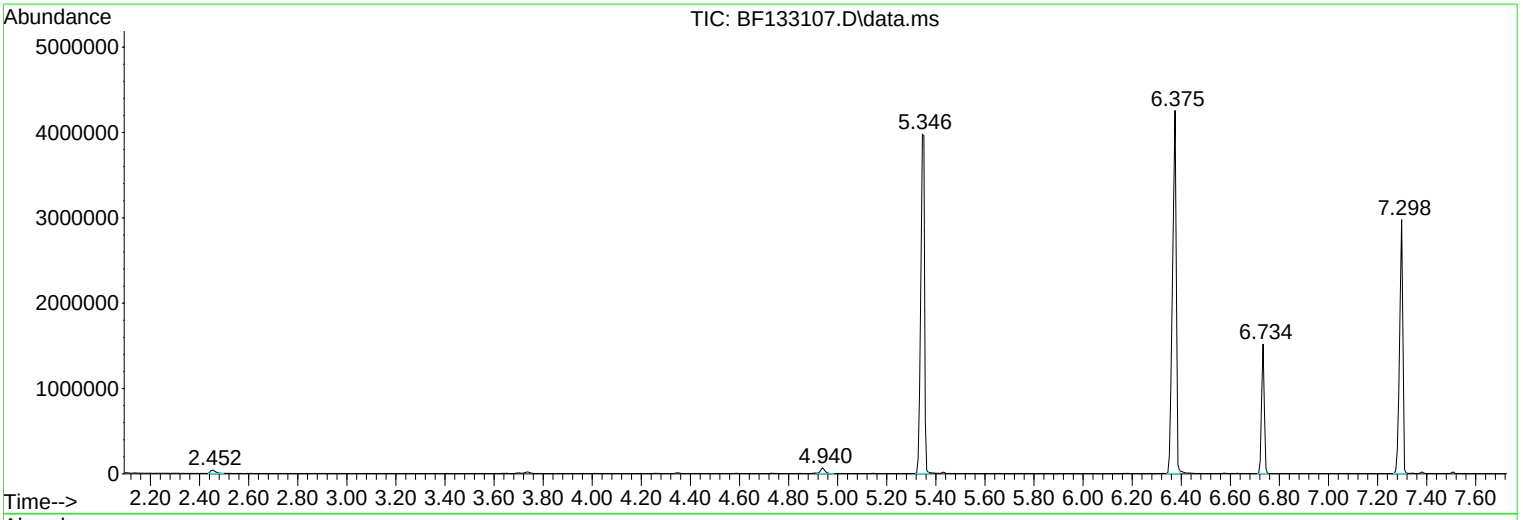
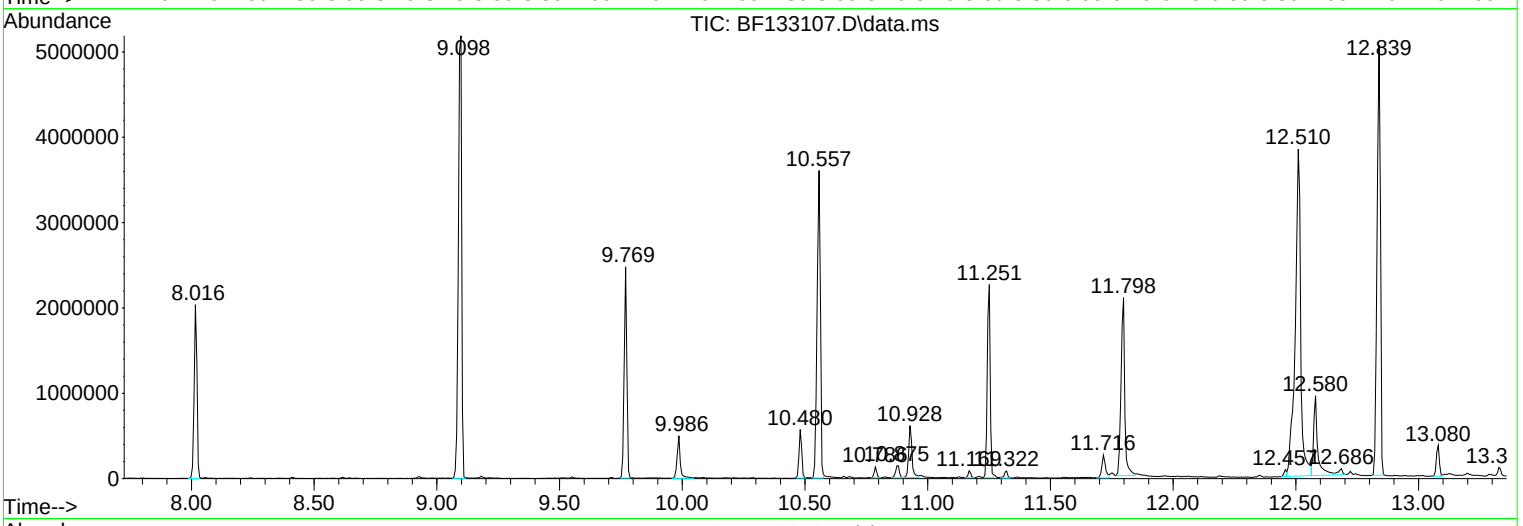
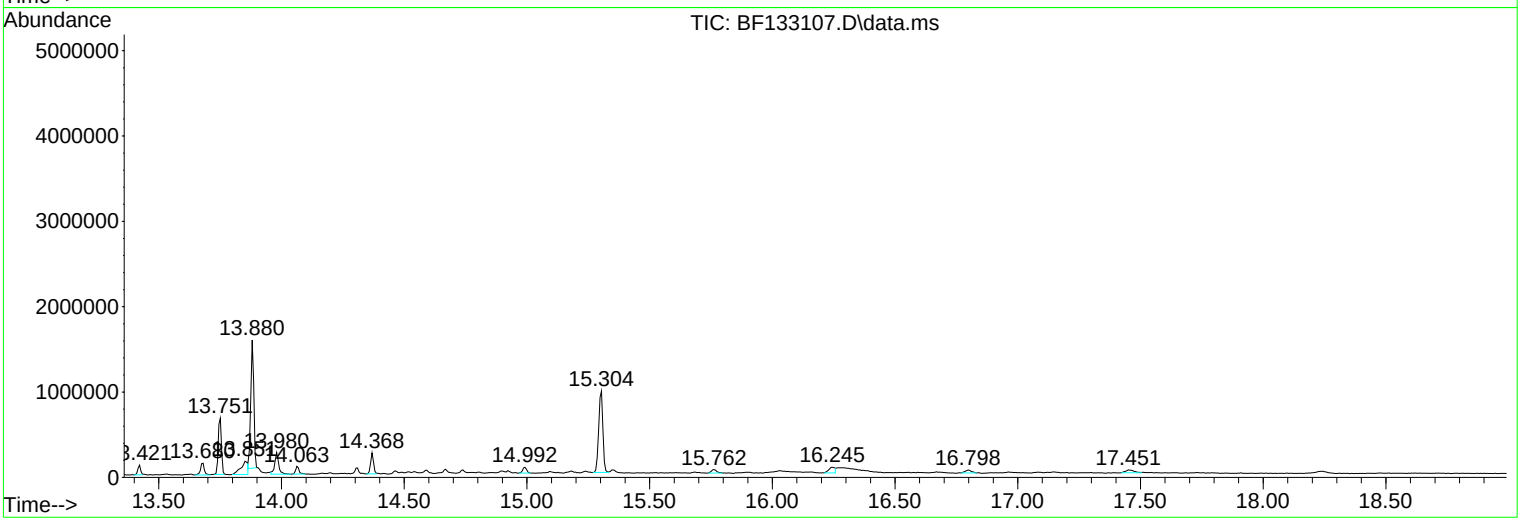
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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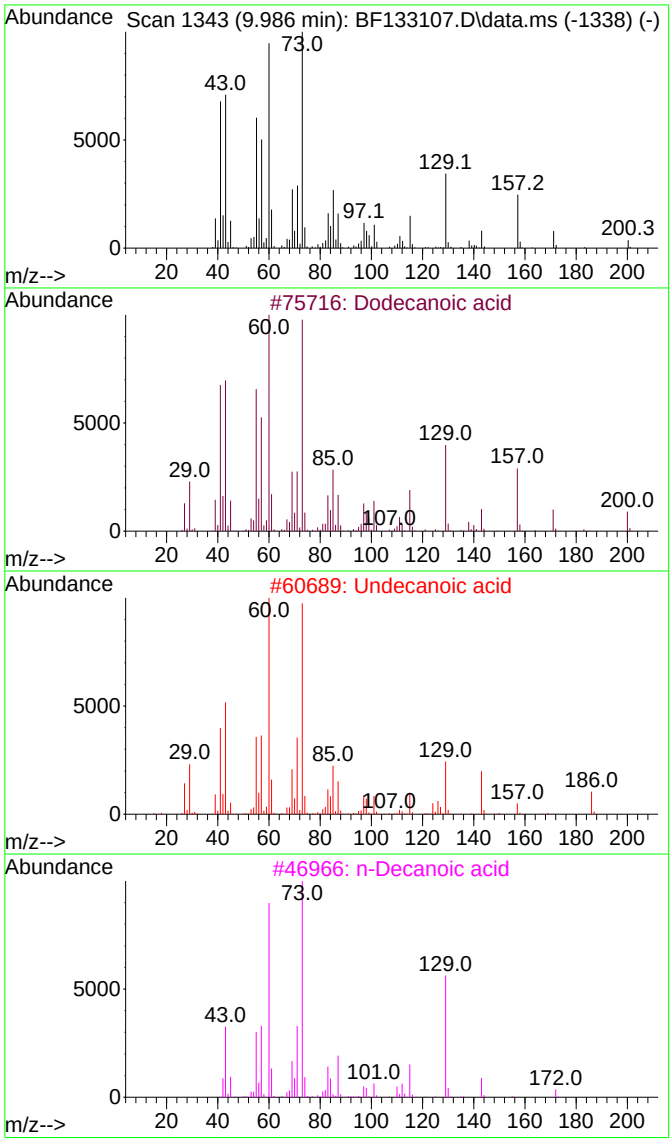
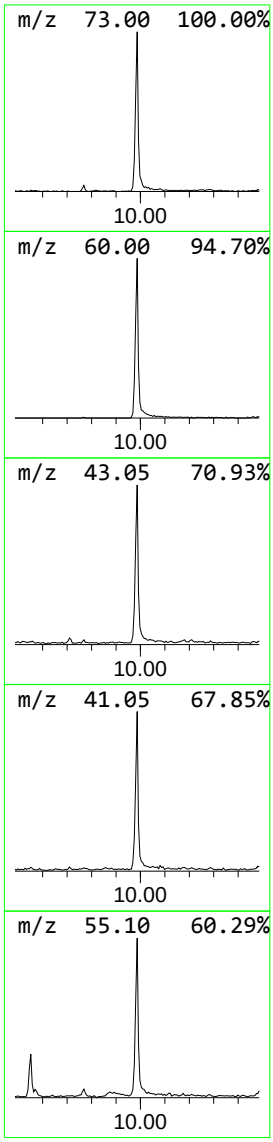
Peak Number 1 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	4.77 ng	447362	Acenaphthene-d10	9.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	96
2	Undecanoic acid	186	C11H22O2	000112-37-8	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Nonanoic acid	158	C9H18O2	000112-05-0	52
5	Hexanoic acid	116	C6H12O2	000142-62-1	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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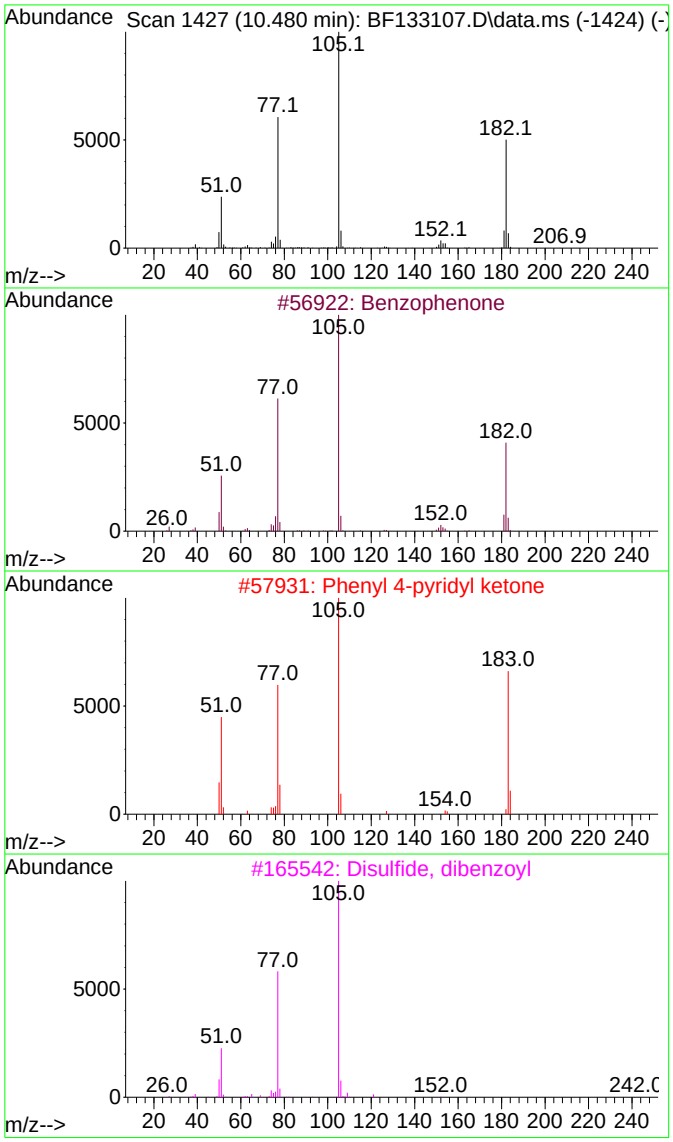
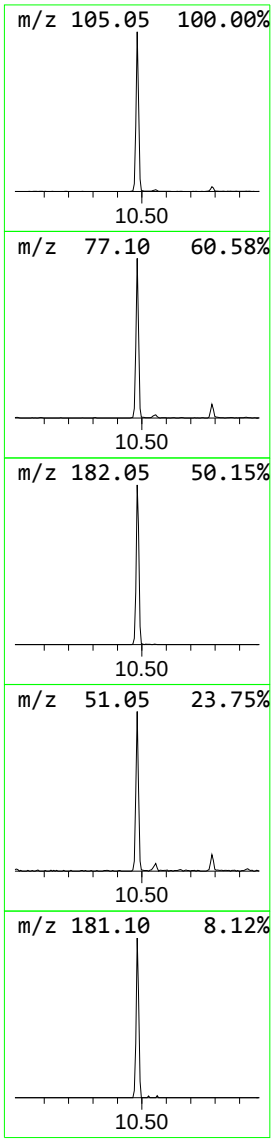
Peak Number 2 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	4.62 ng	433101	Acenaphthene-d10	9.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





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Instrument :
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TR-305A-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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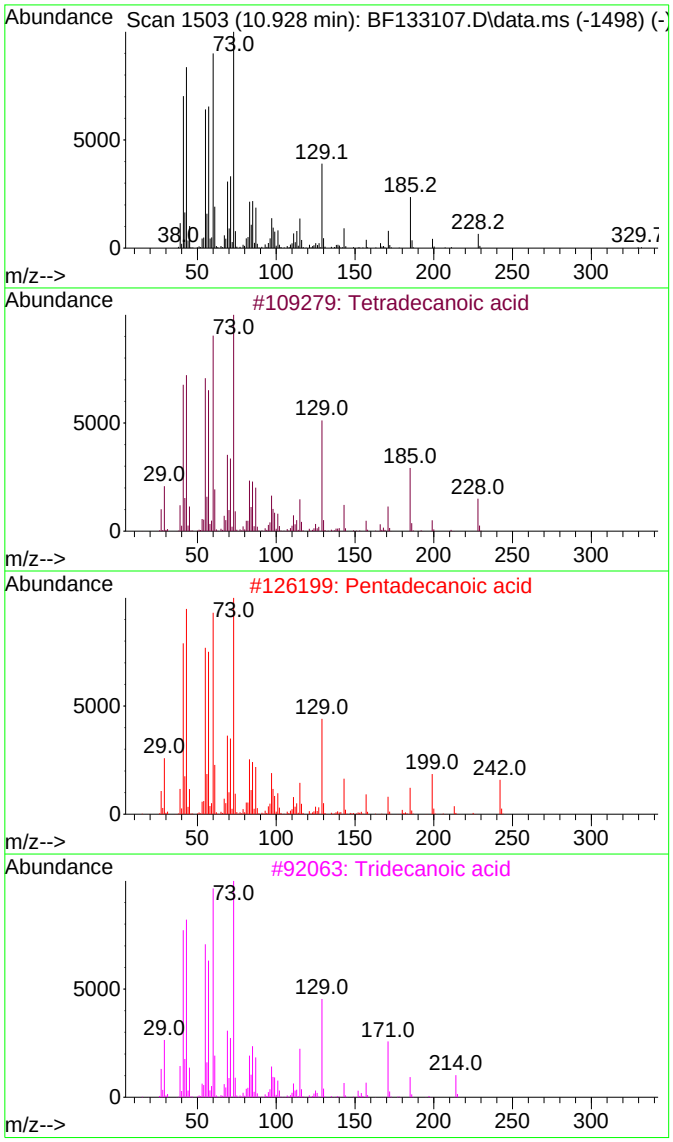
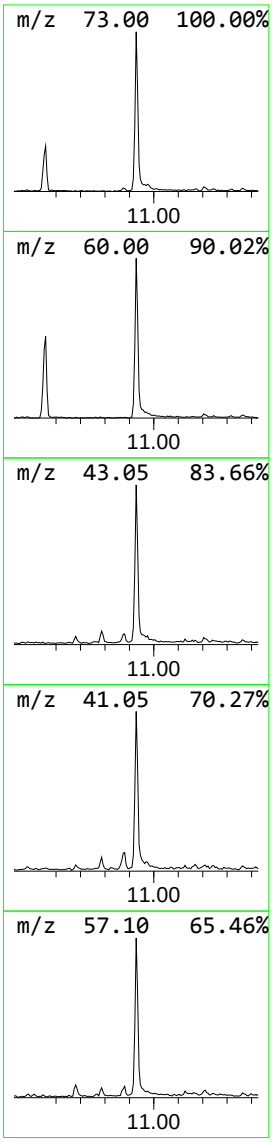
Peak Number 3 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.928	6.01 ng	568405	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	76





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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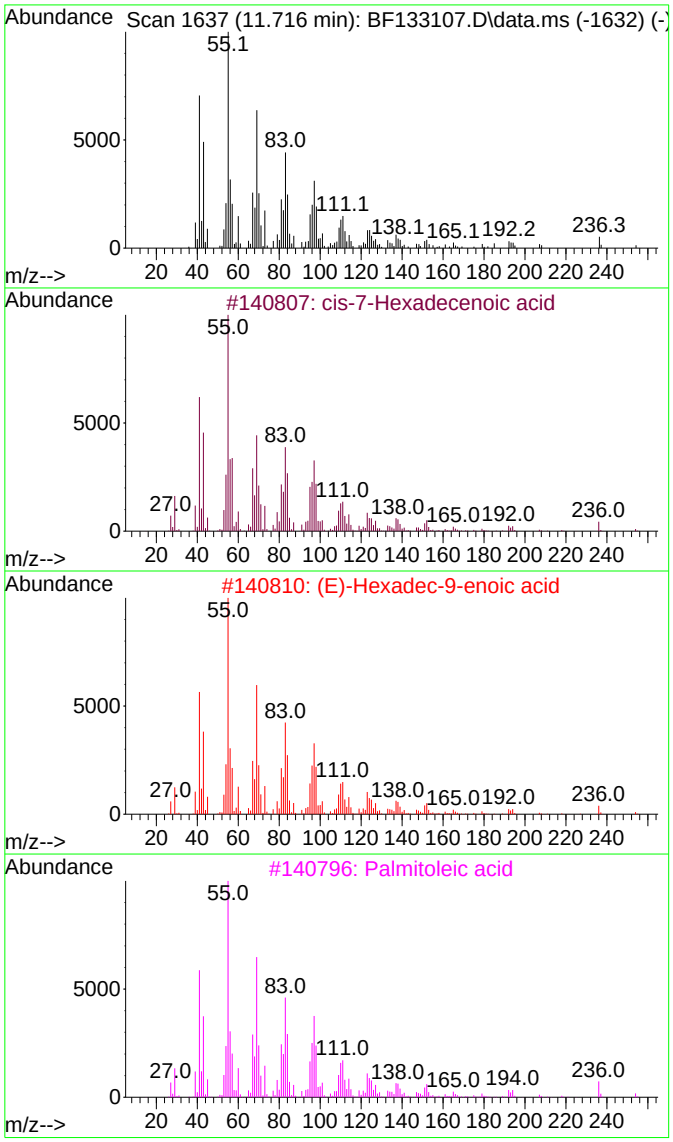
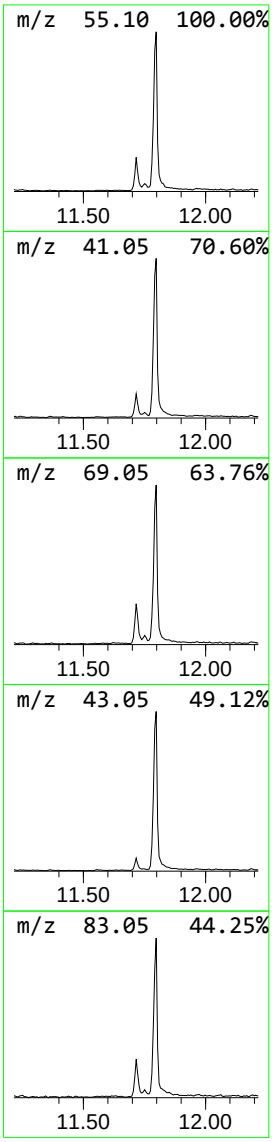
Peak Number 4 cis-7-Hexadecenoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	2.98 ng	282072	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
3	Palmitoleic acid	254	C16H30O2	000373-49-9	99
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	96
5	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	94





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Sample : 02503-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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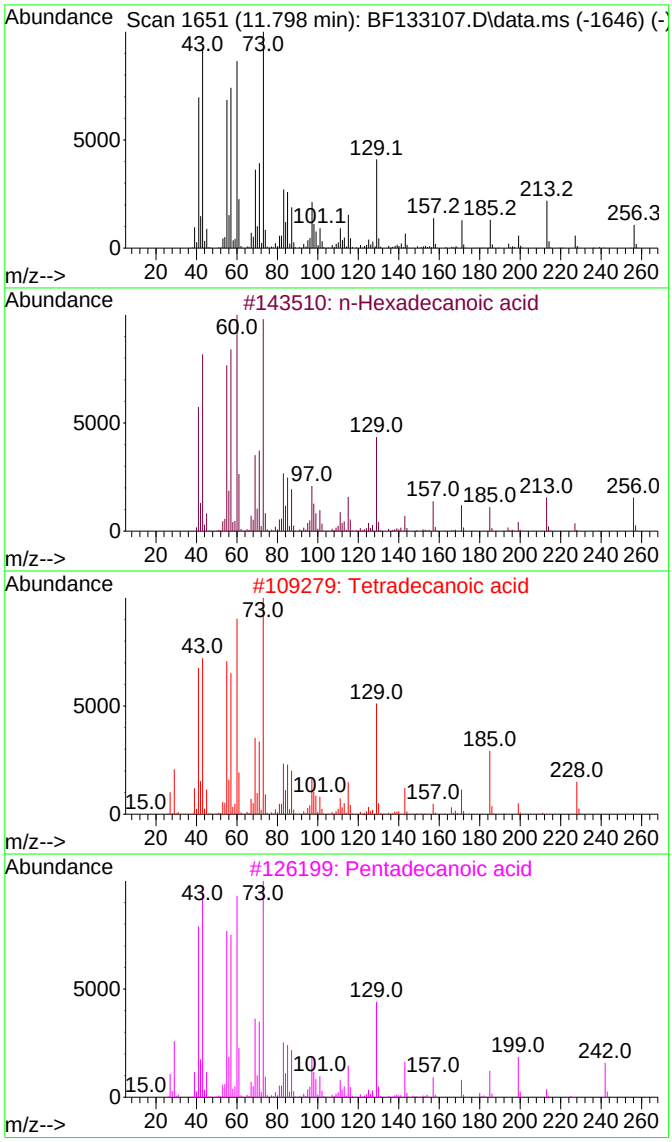
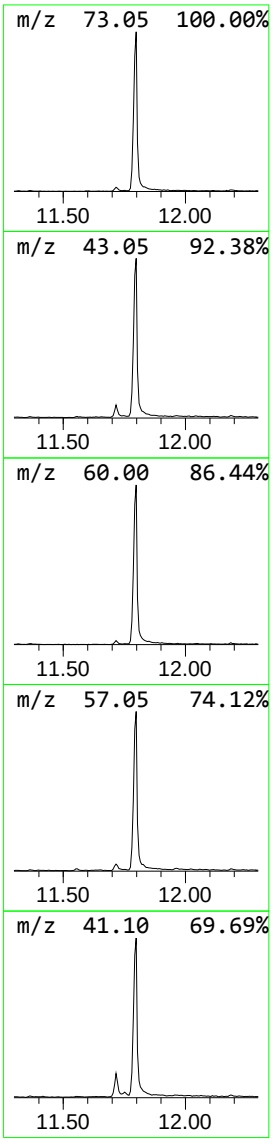
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	23.28 ng	2201050	Phenanthrene-d10	11.251

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	92
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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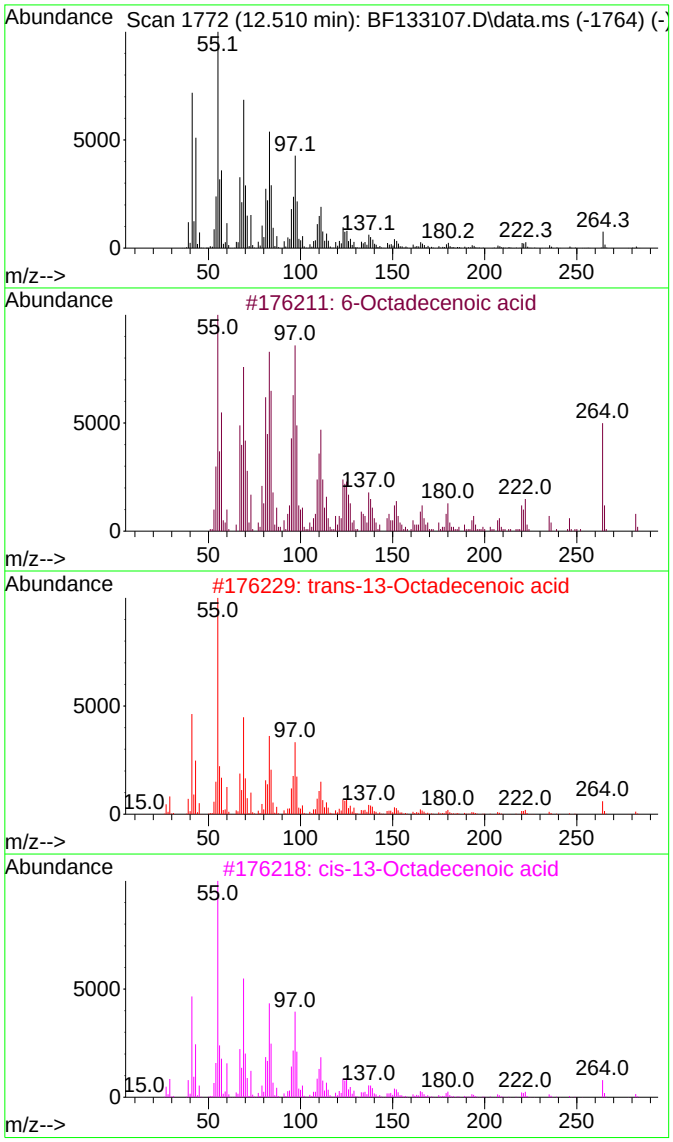
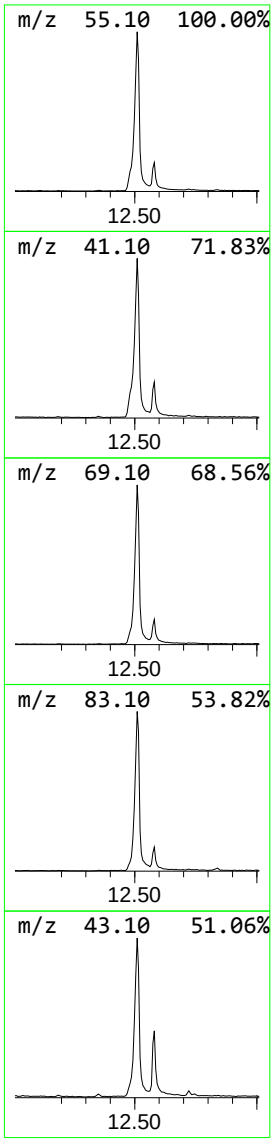
Peak Number 6 6-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	63.66 ng	6019640	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	98
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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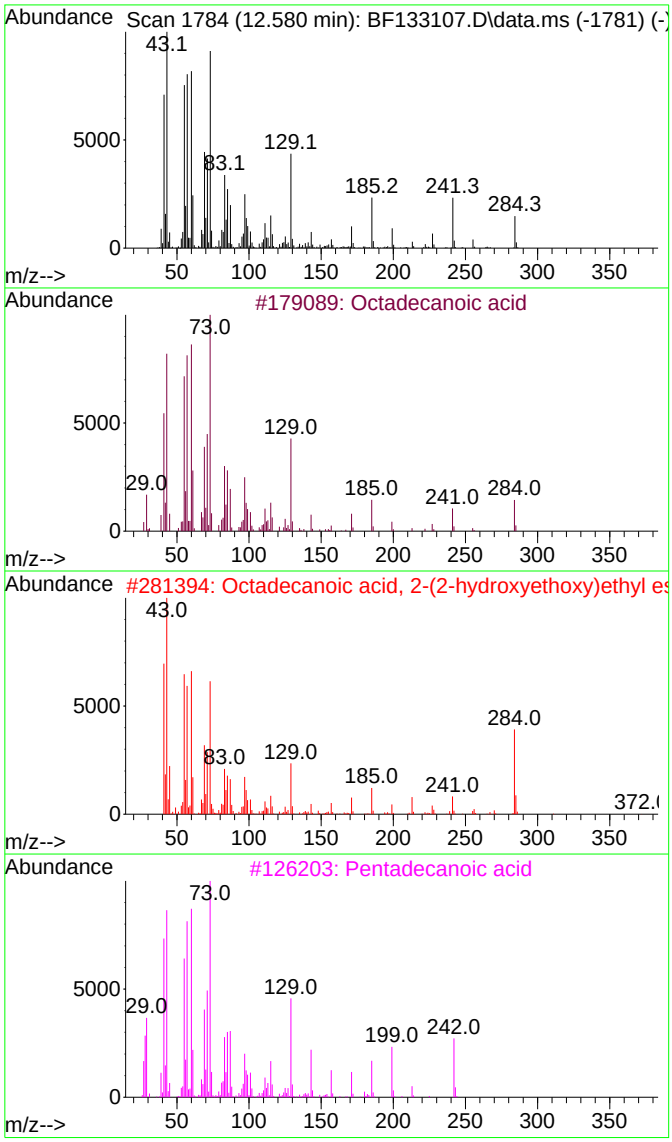
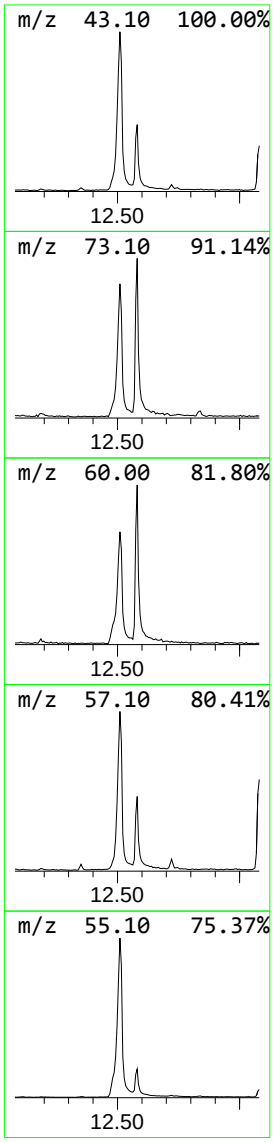
Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	16.13 ng	1061370	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





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Sample : 02503-15
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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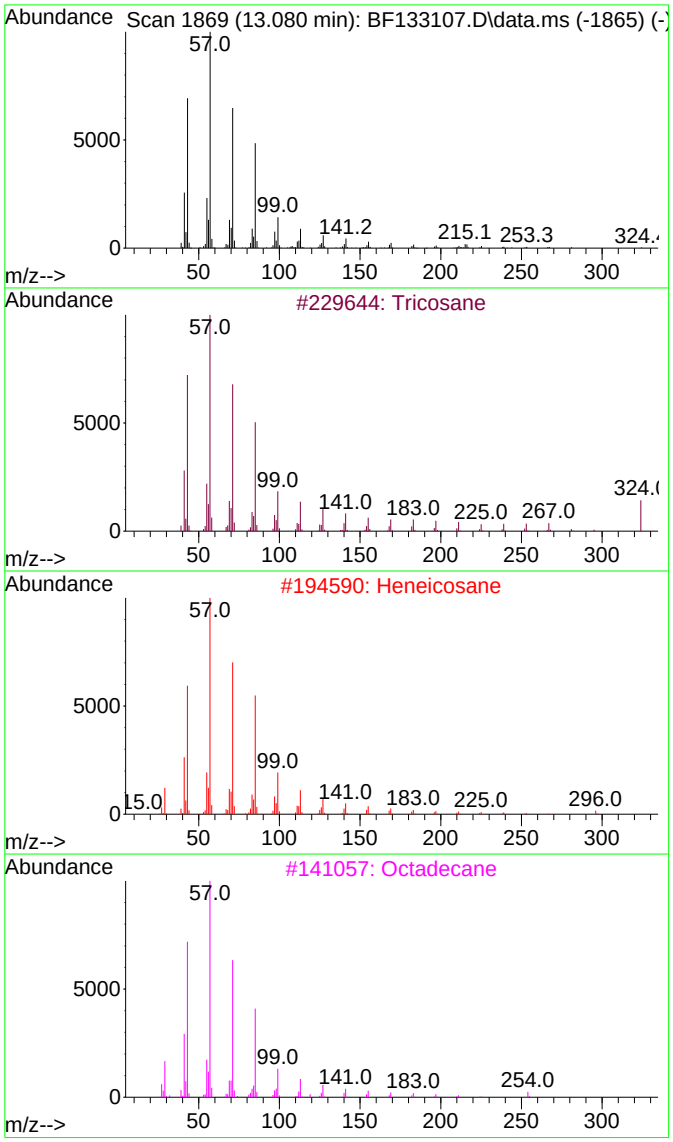
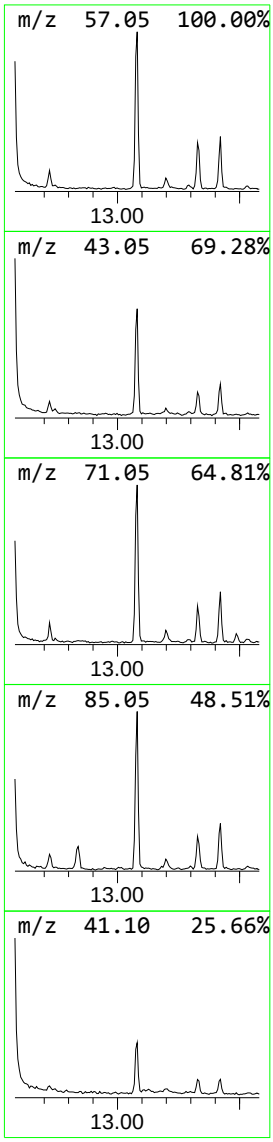
Peak Number 8 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.080	4.68 ng	308144	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	96
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Triacontane	422	C30H62	000638-68-6	91





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Data File : BF133107.D
Acq On : 27 Apr 2023 18:55
Operator : CG\JU
Sample : 02503-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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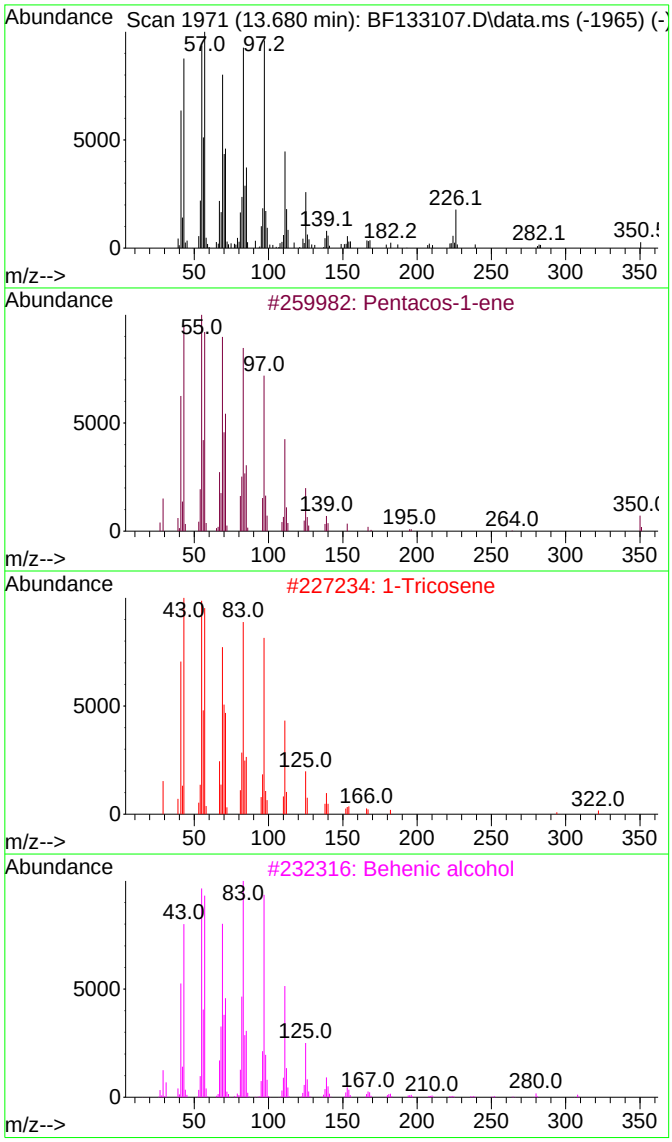
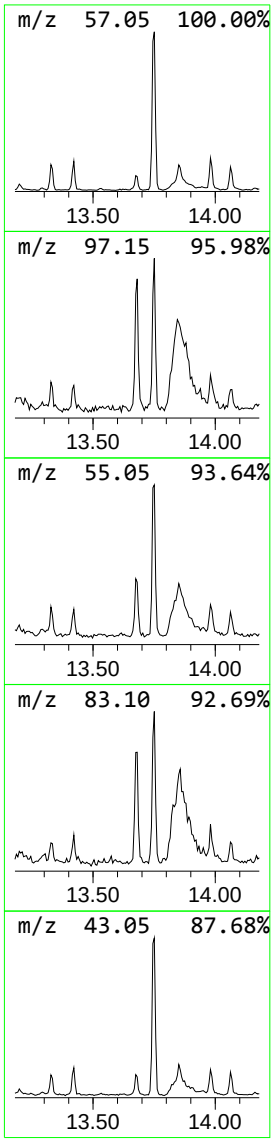
Peak Number 9 Pentacos-1-ene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	2.32 ng	152757	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	99
2	1-Tricosene	322	C23H46	018835-32-0	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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Acq On : 27 Apr 2023 18:55
Operator : CG\JU
Sample : 02503-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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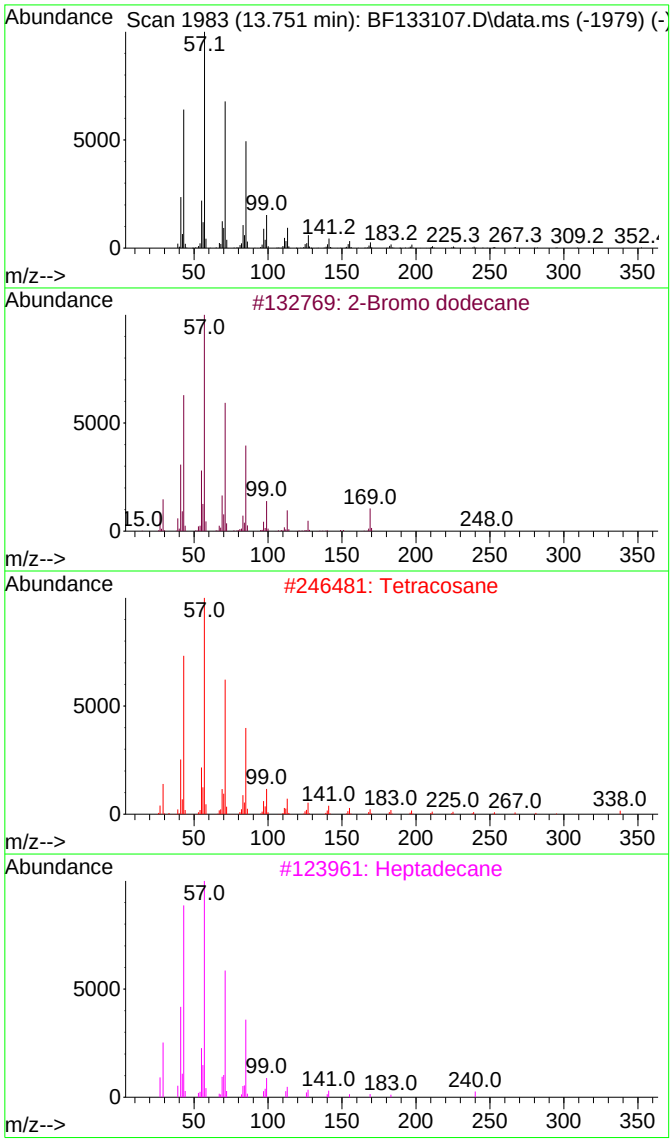
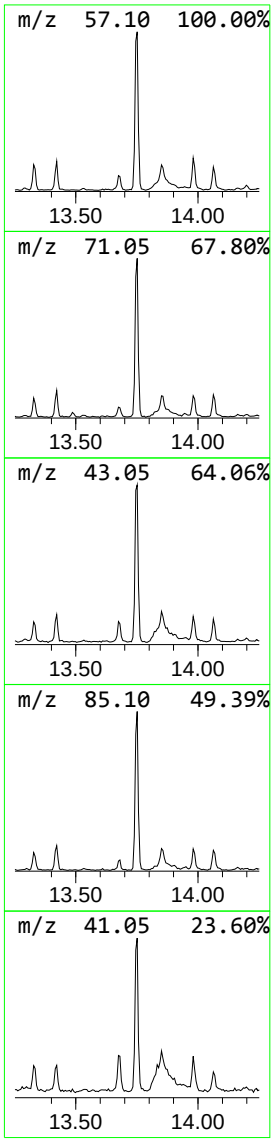
Peak Number 10 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	9.09 ng	597921	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane	282	C20H42	000112-95-8	91





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Data File : BF133107.D
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Operator : CG\JU
Sample : 02503-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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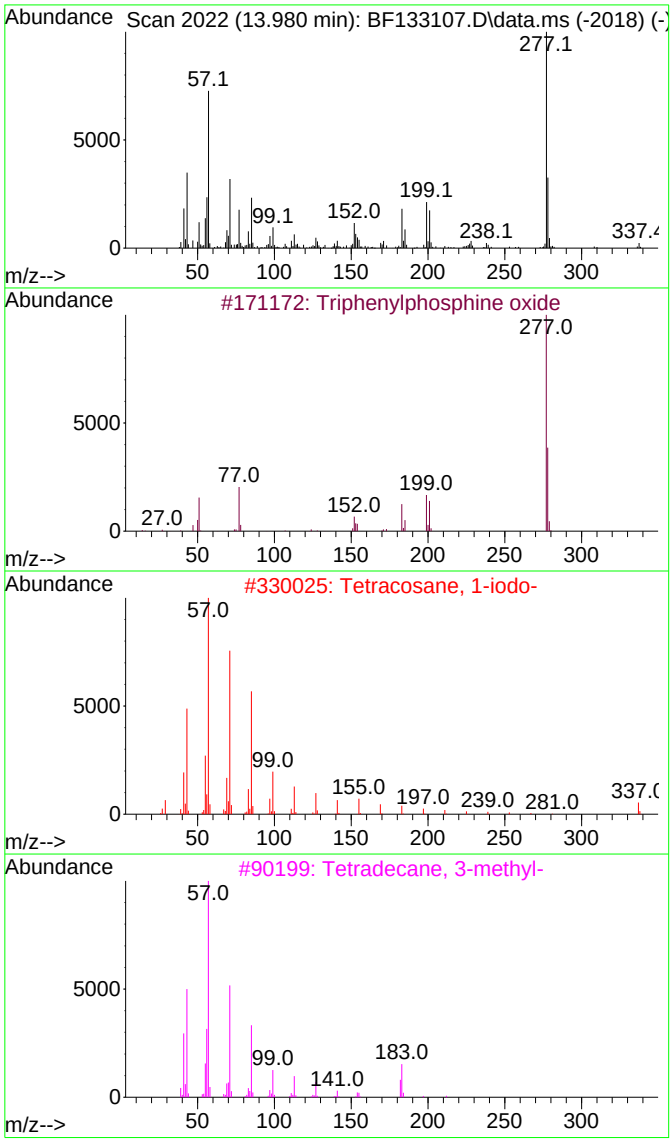
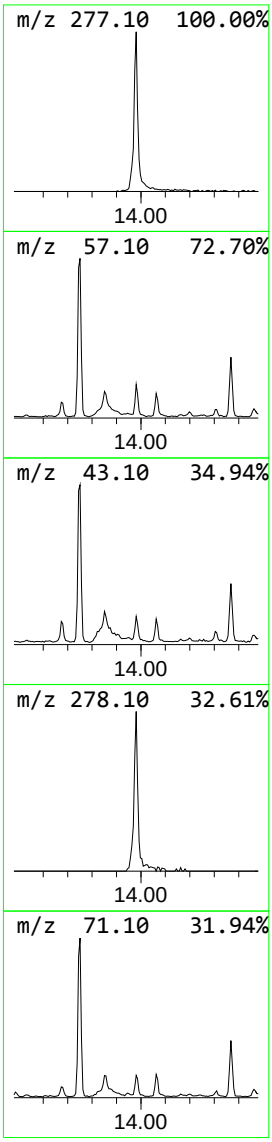
Peak Number 11 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	4.26 ng	280166	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	15
3	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	14
4	Heneicosane, 3-methyl-	310	C22H46	006418-47-9	11
5	Decane, 3-methyl-	156	C11H24	013151-34-3	11





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Sample : 02503-15
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
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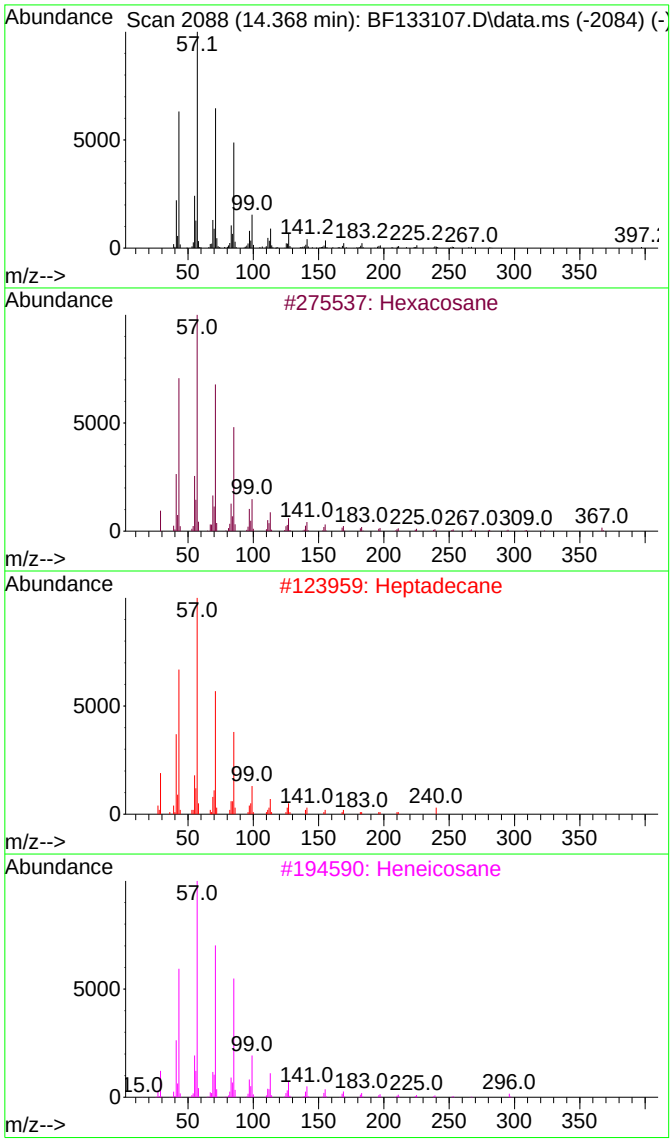
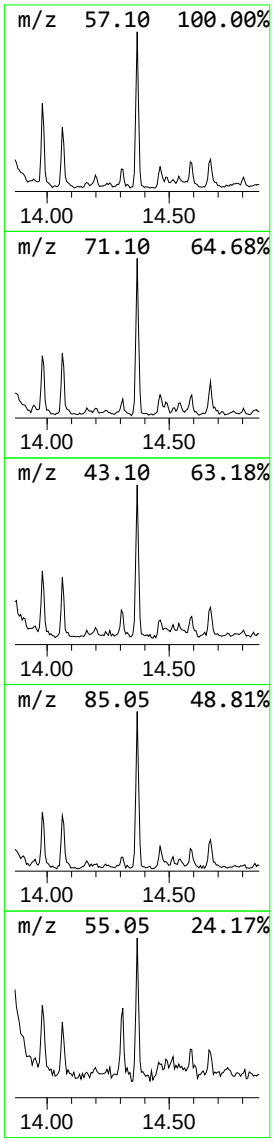
Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	3.17 ng	208271	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heptadecane	240	C17H36	000629-78-7	94
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	91
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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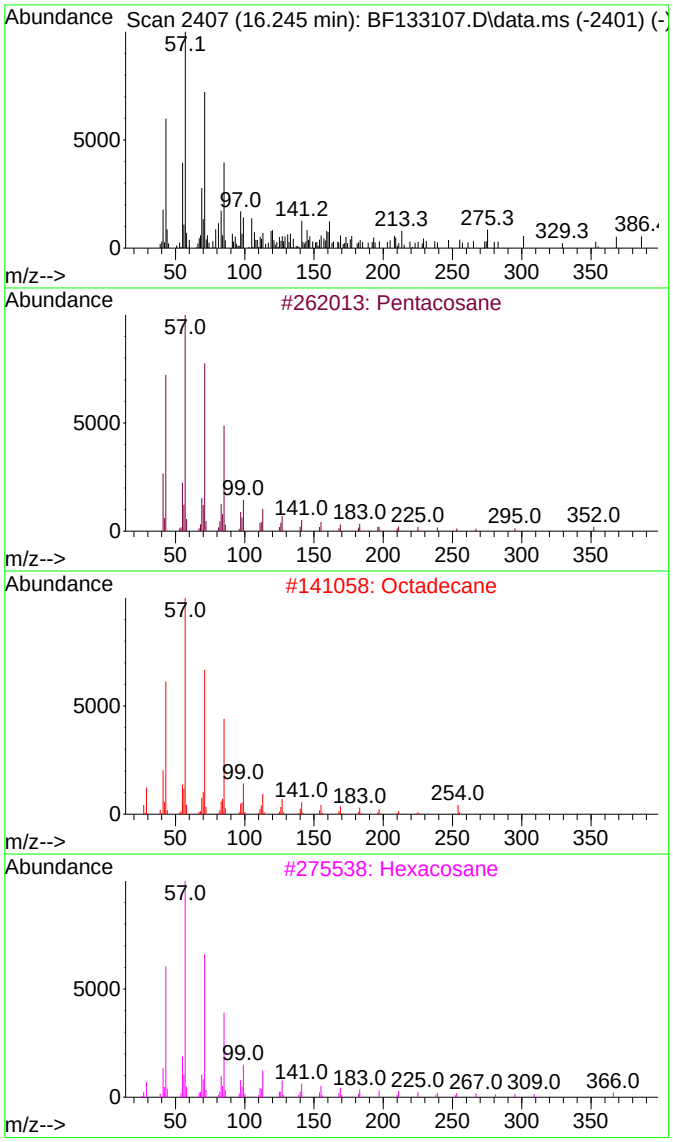
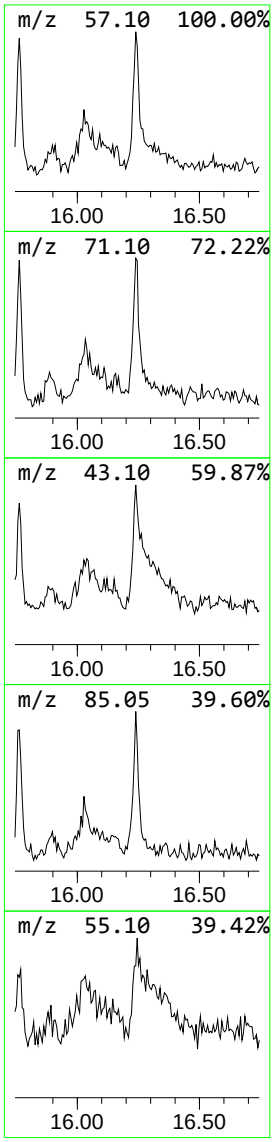
Peak Number 13 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	2.16 ng	122283	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	64
2	Octadecane	254	C18H38	000593-45-3	58
3	Hexacosane	366	C26H54	000630-01-3	58
4	Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	58
5	Tetracosane	338	C24H50	000646-31-1	58





Tentatively Identified Compound (LSC) summary

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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
Dodecanoic acid	9.986	4.8	ng	447362	3	9.769	1874230	20.0
Benzophenone	10.480	4.6	ng	433101	3	9.769	1874230	20.0
Tetradecanoic acid	10.928	6.0	ng	568405	4	11.251	1891120	20.0
cis-7-Hexadecen...	11.716	3.0	ng	282072	4	11.251	1891120	20.0
n-Hexadecanoic ...	11.798	23.3	ng	2201050	4	11.251	1891120	20.0
6-Octadecenoic ...	12.510	63.7	ng	6019640	4	11.251	1891120	20.0
Octadecanoic acid	12.580	16.1	ng	1061370	5	13.880	1315700	20.0
Tricosane	13.080	4.7	ng	308144	5	13.880	1315700	20.0
Pentacos-1-ene	13.680	2.3	ng	152757	5	13.880	1315700	20.0
2-Bromo dodecane	13.751	9.1	ng	597921	5	13.880	1315700	20.0
Triphenylphosph...	13.980	4.3	ng	280166	5	13.880	1315700	20.0
Hexacosane	14.368	3.2	ng	208271	5	13.880	1315700	20.0
Pentacosane	16.245	2.2	ng	122283	6	15.304	1130020	20.0