LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.598	593	597	615	rBV	100877	328413	8.83%	1.749%
2	6.598	763	767	787	rBV	138773	490280	13.18%	2.611%
3	6.734	787	790	811	rVB	311260	581534	15.64%	3.097%
4	6.963	826	829	849	rBV	376530	668389	17.97%	3.559%
5	7.116	852	855	869	rVV	321884	432044	11.62%	2.301%
6	7.534	922	926	940	rBV2	119813	332994	8.95%	1.773%
7	8.245	1044	1047	1058	rBV	651612	871516	23.43%	4.641%
8	8.745	1127	1132	1135	rBV3	31646	38836	1.04%	0.207%
9	8.816	1140	1144	1148	rVV2	41834	43454	1.17%	0.231%
10	9.063	1183	1186	1190	rBV3	40433	49335	1.33%	0.263%
11	9.316	1225	1229	1238	rBV	588217	714447	19.21%	3.804%
12	9.380	1238	1240	1246	rVB	81111	78861	2.12%	0.420%
13	9.704	1291	1295	1303	rVB2	64243	109487	2.94%	0.583%
14	9.910	1327	1330	1335	rVB	94066	82327	2.21%	0.438%
15	10.004	1342	1346	1351	rBV	921131	920428	24.75%	4.901%
16	10.410	1410	1415	1418	rBV2	120164	117302	3.15%	0.625%
17	10.557	1433	1440	1447	rBV	42564	82946	2.23%	0.442%
18	10.633	1448	1453	1455	rBV	44413	54353	1.46%	0.289%
19	10.798	1477	1481	1493	rBV	247042	367350	9.88%	1.956%
20	10.886	1493	1496	1505	rVB	114137	146165	3.93%	0.778%
21	11.333	1569	1572	1575	rBV	78648	68629	1.85%	0.365%
22	11.498	1597	1600	1603	rBV	659520	736997	19.82%	3.924%
23	11.522	1603	1604	1611	rVV	259108	287125	7.72%	1.529%
24	11.580	1611	1614	1617	rVV	43215	47350	1.27%	0.252%
25	11.763	1642	1645	1648	rVB	66510	54395	1.46%	0.290%
26	11.869	1659	1663	1669	rBV	1290136	1141822	30.70%	6.080%
27	12.004	1683	1686	1688	rBV	46491	56466	1.52%	0.301%
28	12.033	1688	1691	1697	rVB2	47075	64345	1.73%	0.343%
29	12.116	1702	1705	1708	rVV2	67122	91059	2.45%	0.485%
30	12.169	1712	1714	1722	rVB	55719	63202	1.70%	0.337%
31	12.563	1776	1781	1782	rBV	3729333	3719114	100.00%	19.804%
32	12.580	1782	1784	1792	rVV2	2655455	2718627	73.10%	14.476%
33	12.663	1794	1798	1803	rVV	484938	505581	13.59%	2.692%
34	12.721	1804	1808	1822	rVB	218153	300302	8.07%	1.599%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.933	1841	1844	1845	rBV	77854	72448	1.95%	0.386%
36	12.951	1845	1847	1853	rVB	214630	227185	6.11%	1.210%
37	13.080	1866	1869	1877	rBV	475091	492290	13.24%	2.621%
38	13.386	1918	1921	1924	rBV2	63184	56163	1.51%	0.299%
39	13.963	2016	2019	2023	rVB3	54878	52924	1.42%	0.282%
40	14.057	2033	2035	2041	rBV2	42201	58075	1.56%	0.309%
41	14.157	2047	2052	2064	rBV2	595098	900564	24.21%	4.795%
42	15.704	2311	2315	2326	rVB2	300897	554756	14.92%	2.954%

Sum of corrected areas: 18779880

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
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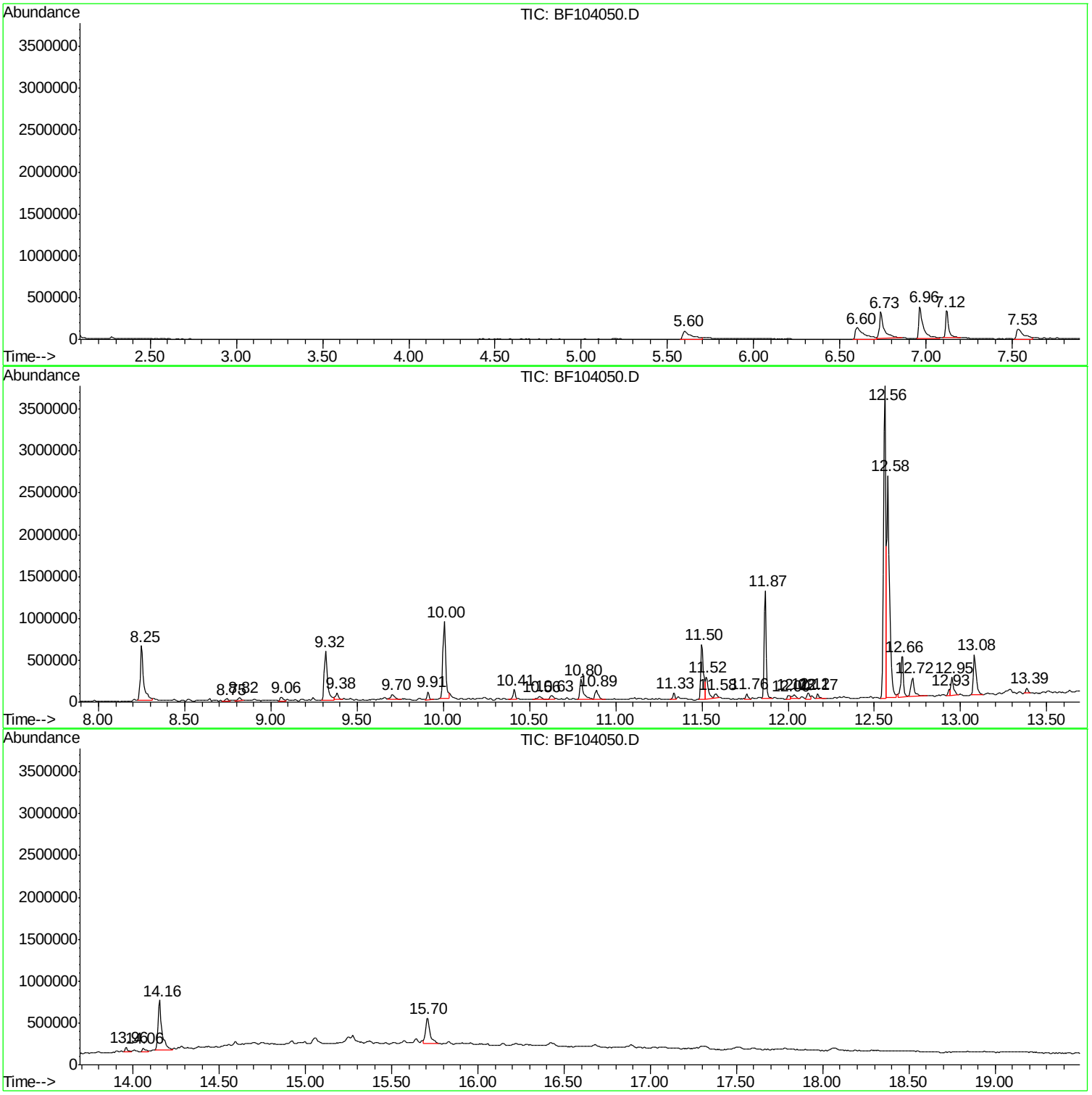
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
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Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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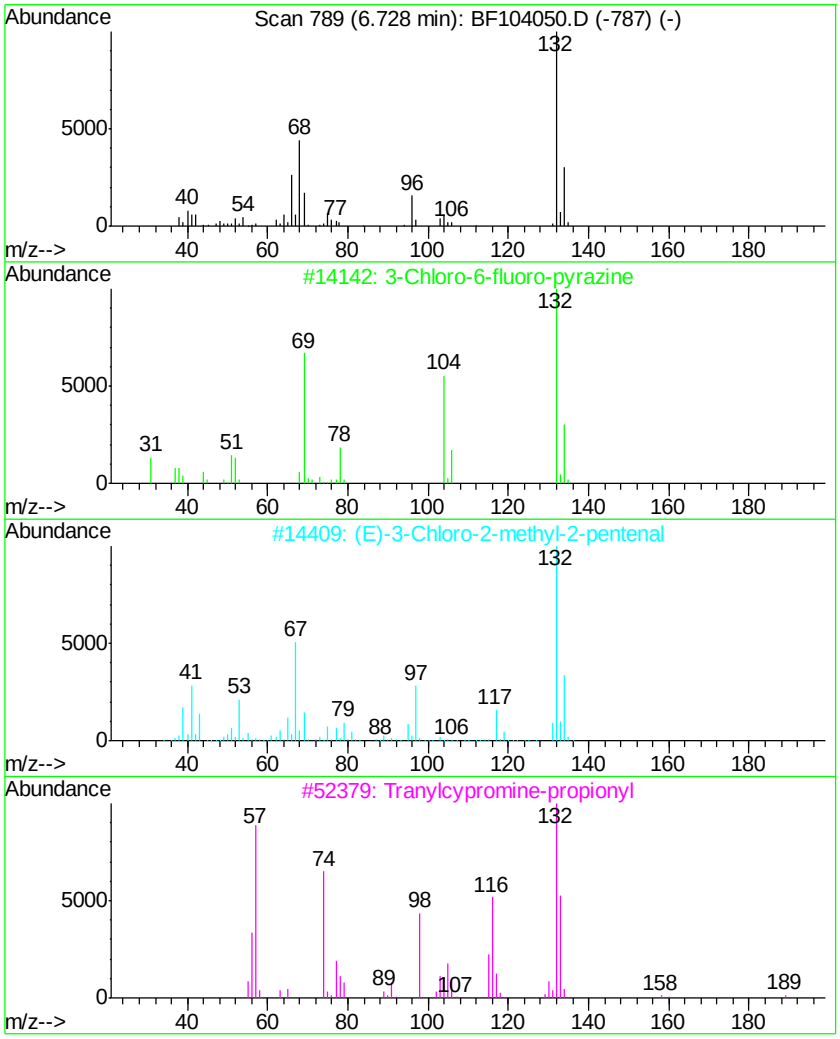
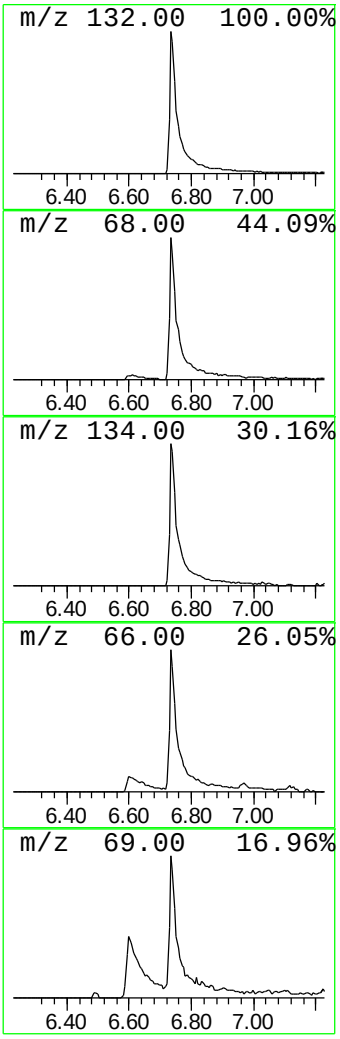
Peak Number 1 unknown6.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	17.40 ng	581534	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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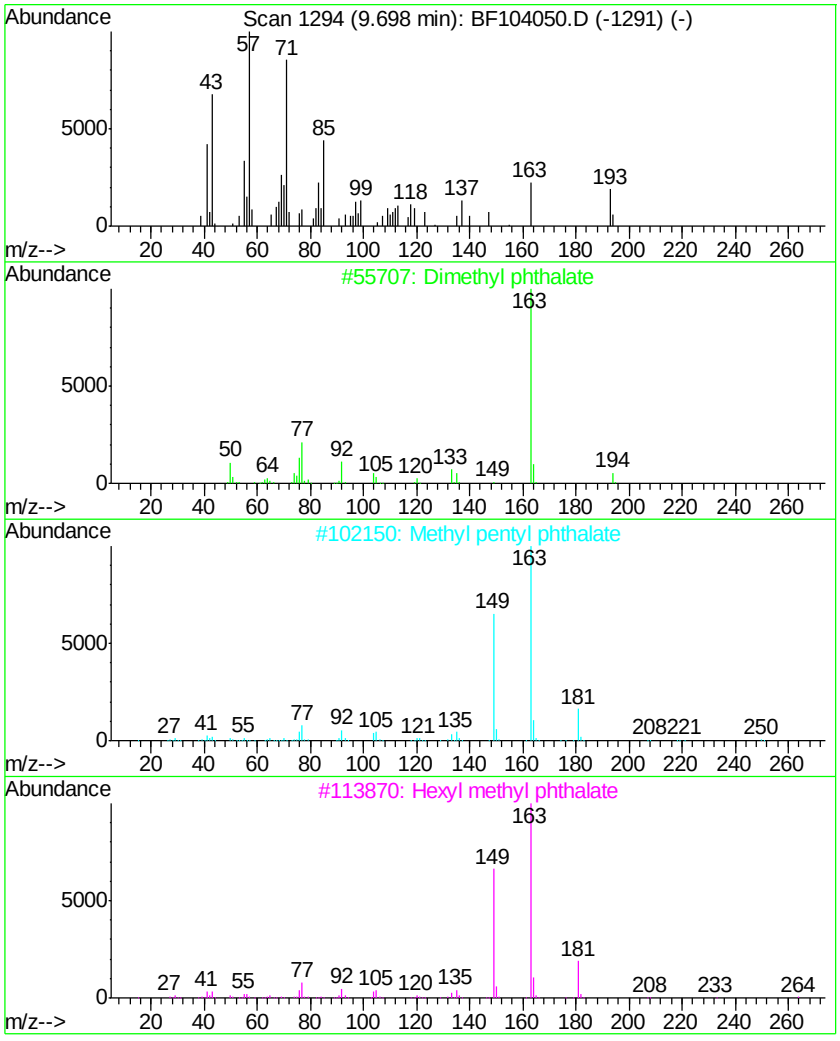
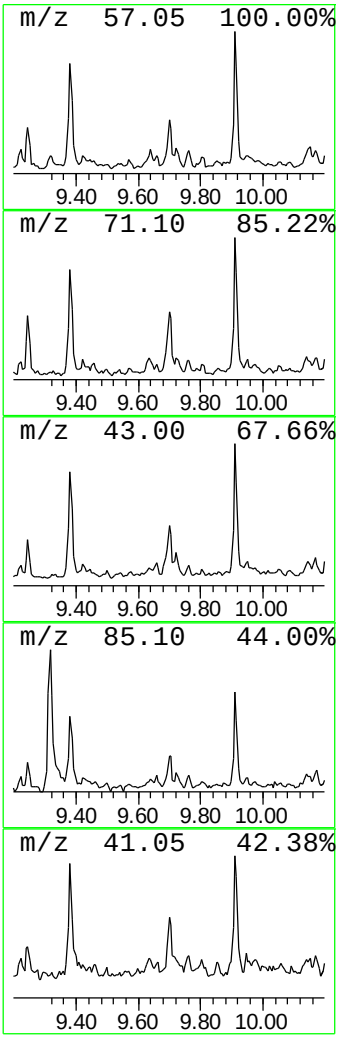
Peak Number 3 Dimethyl phthalate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	2.38 ng	109487	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl phthalate	194	C10H10O4	000131-11-3	95
2	Methyl pentyl phthalate	250	C14H18O4	1000373-89-5	43
3	Hexyl methyl phthalate	264	C15H20O4	1000373-89-7	43
4	Heptyl methyl phthalate	278	C16H22O4	1000373-88-4	43
5	Methyl octyl phthalate	292	C17H24O4	091485-83-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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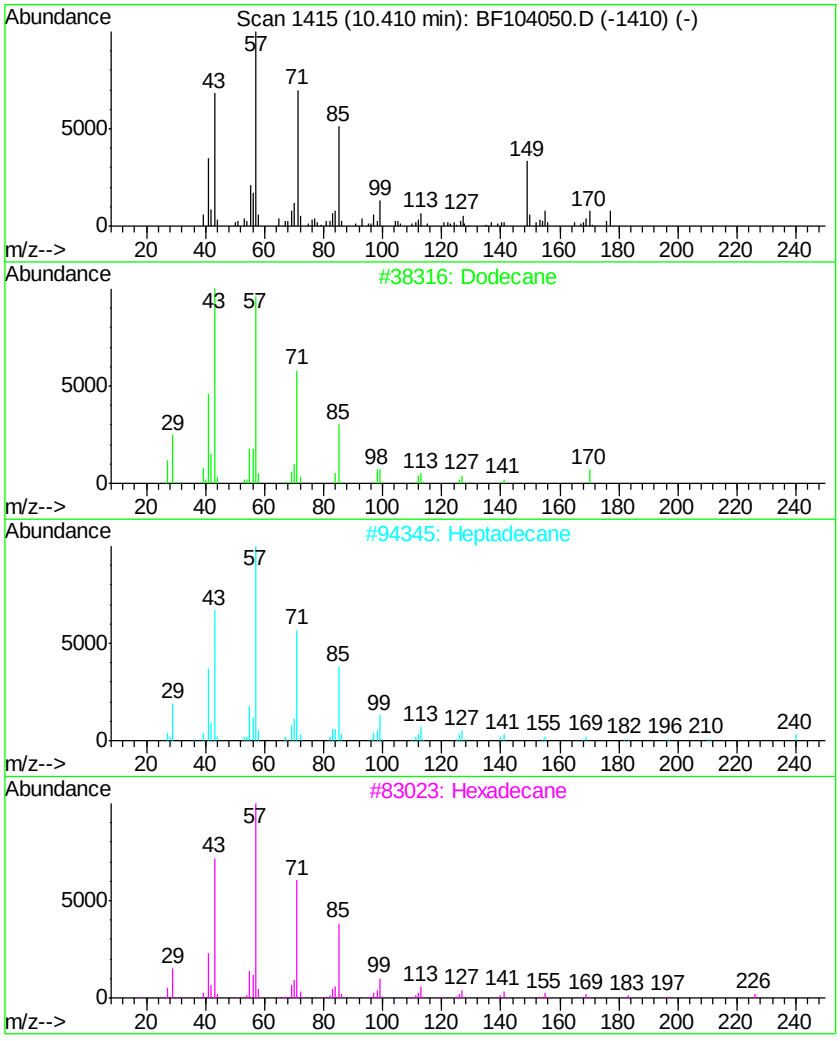
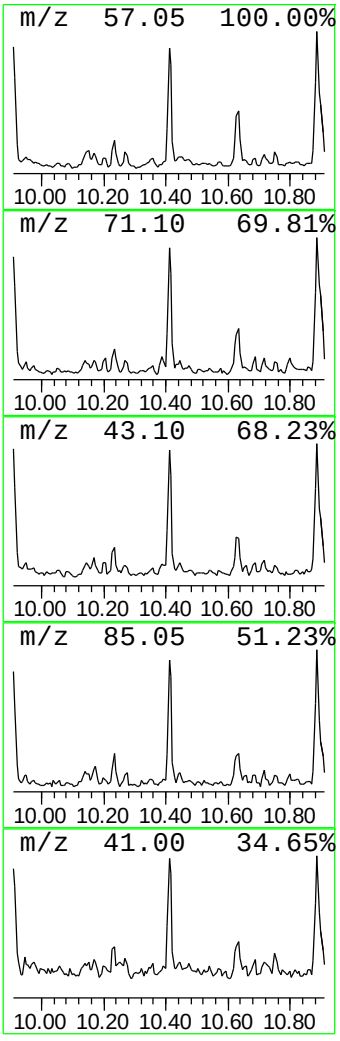
Peak Number 4 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	2.55 ng	117302	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	89
2	Heptadecane	240	C17H36	000629-78-7	64
3	Hexadecane	226	C16H34	000544-76-3	59
4	Tetradecane	198	C14H30	000629-59-4	58
5	Tetracosane	338	C24H50	000646-31-1	58





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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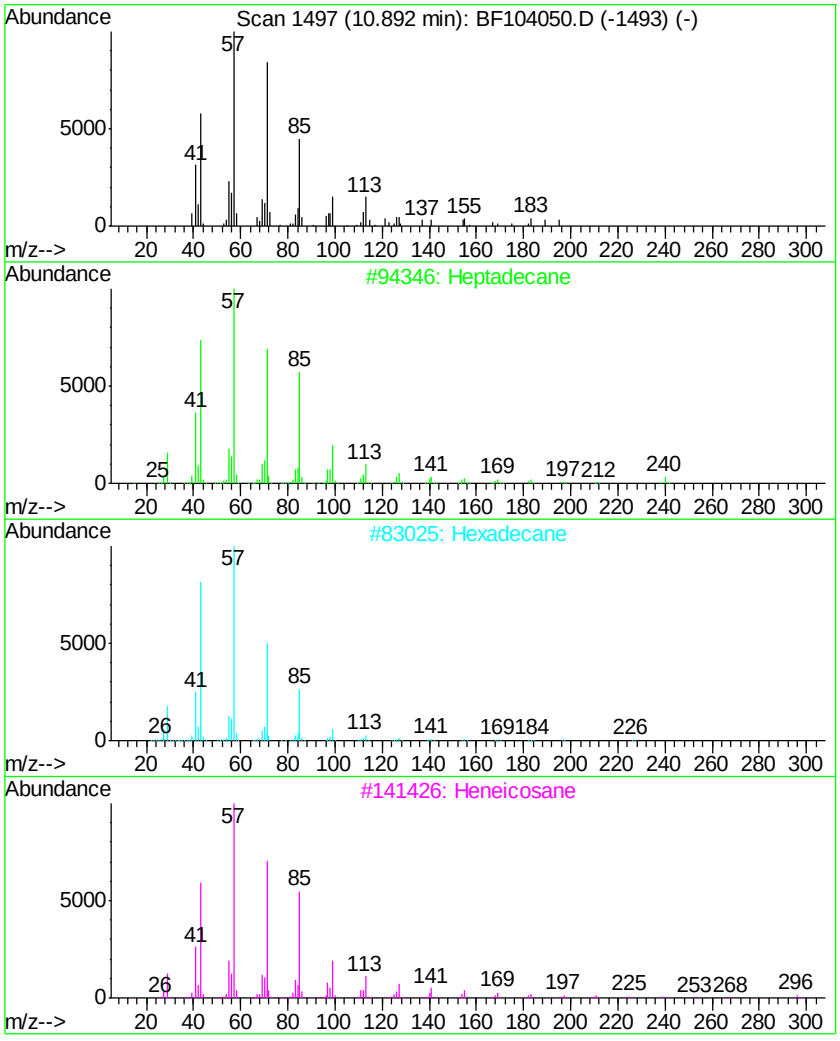
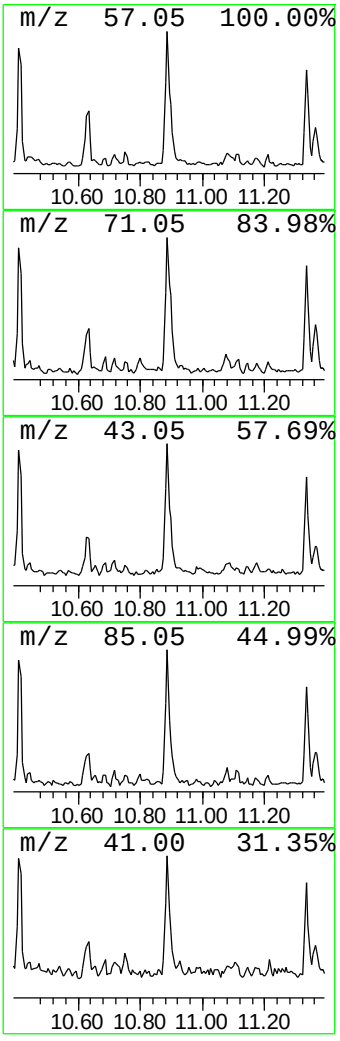
Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	3.97 ng	146165	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Nonadecane	268	C19H40	000629-92-5	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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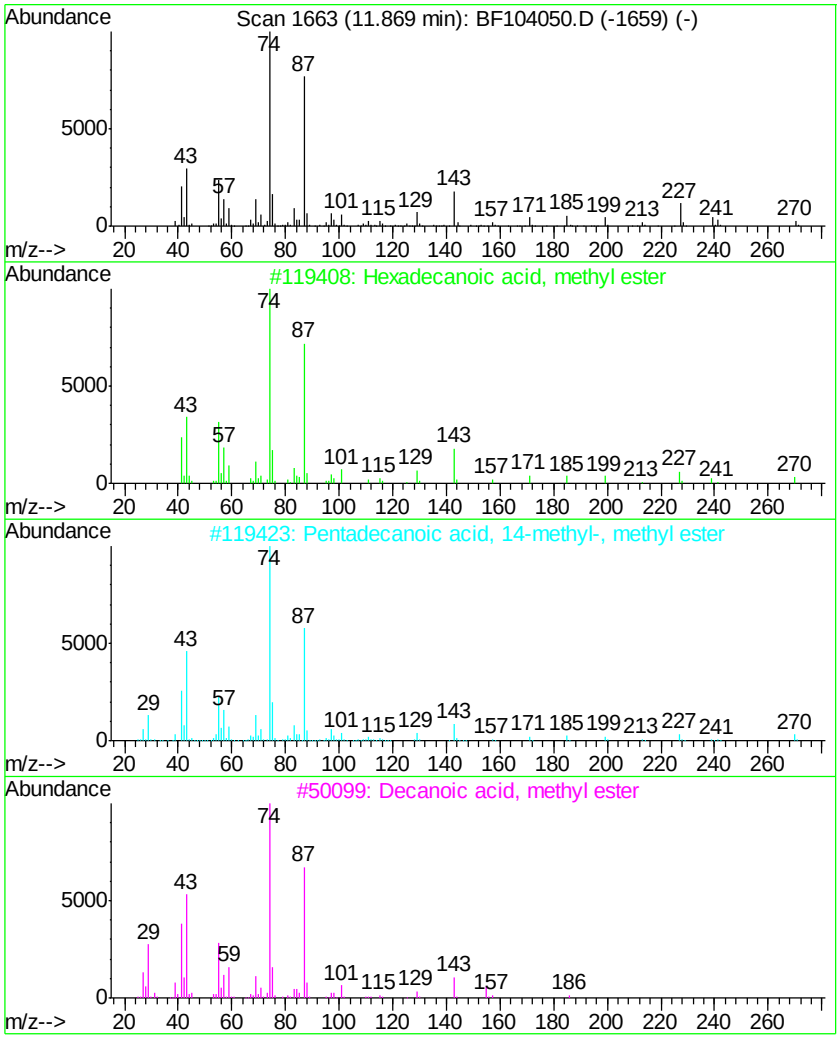
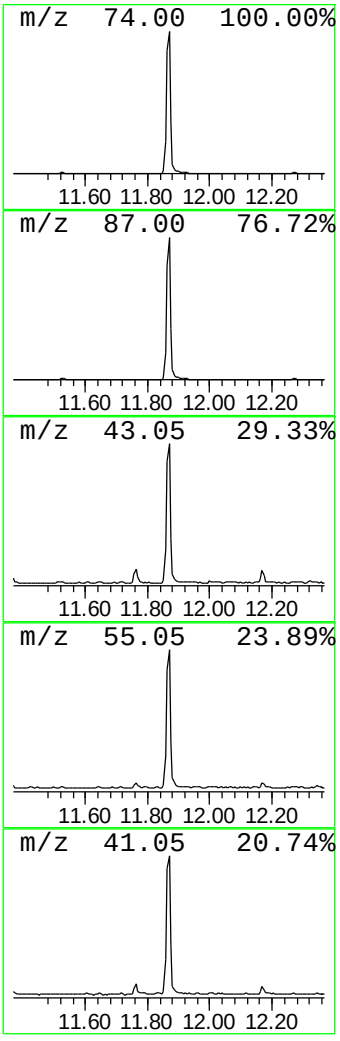
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	30.99 ng	1141820	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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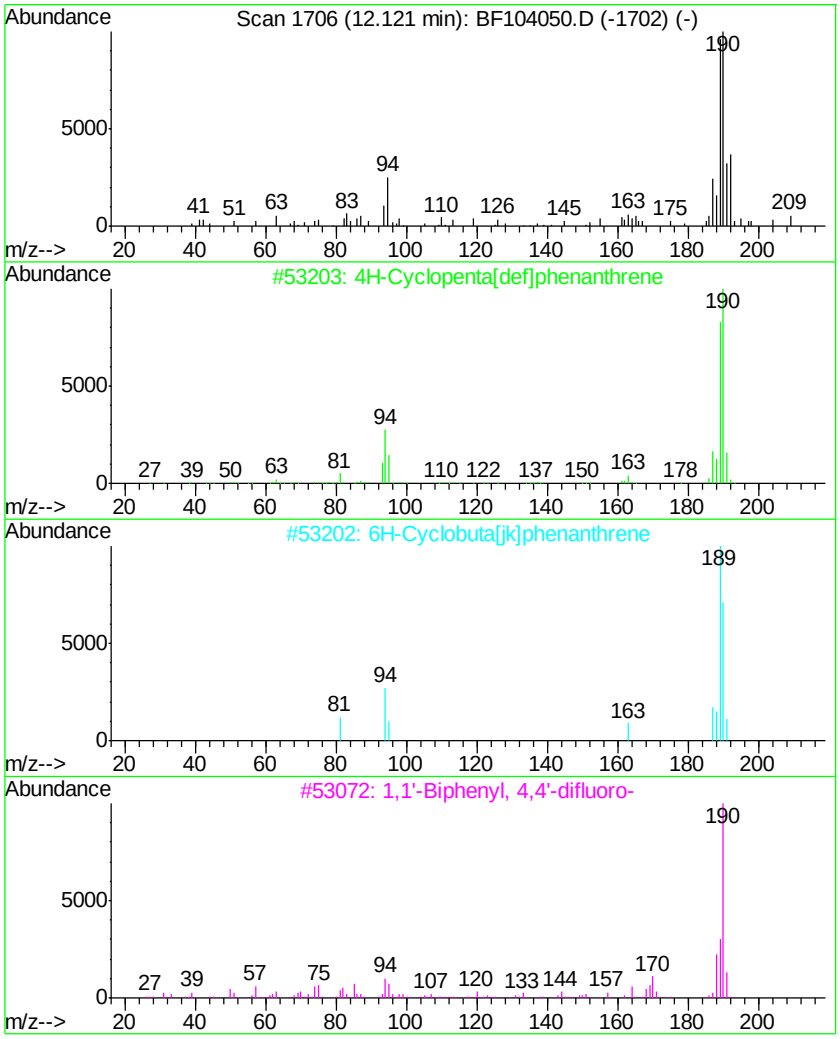
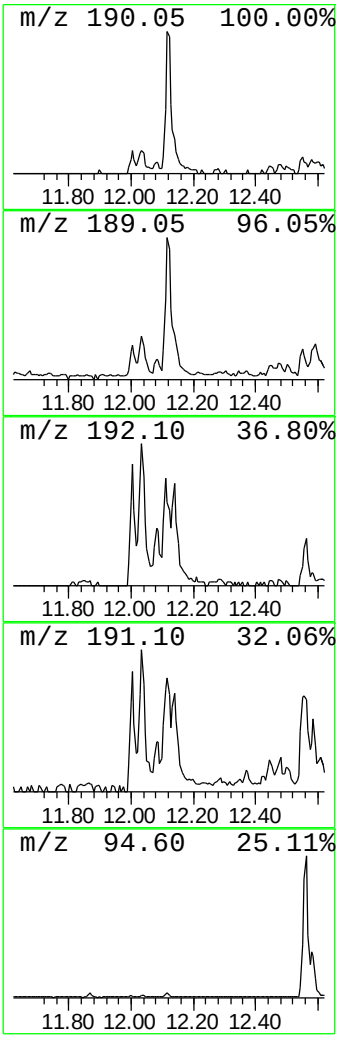
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	2.47 ng	91059	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	32
4	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	25
5	Methyl diselenide	190	C2H6Se2	007101-31-7	25





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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-032718-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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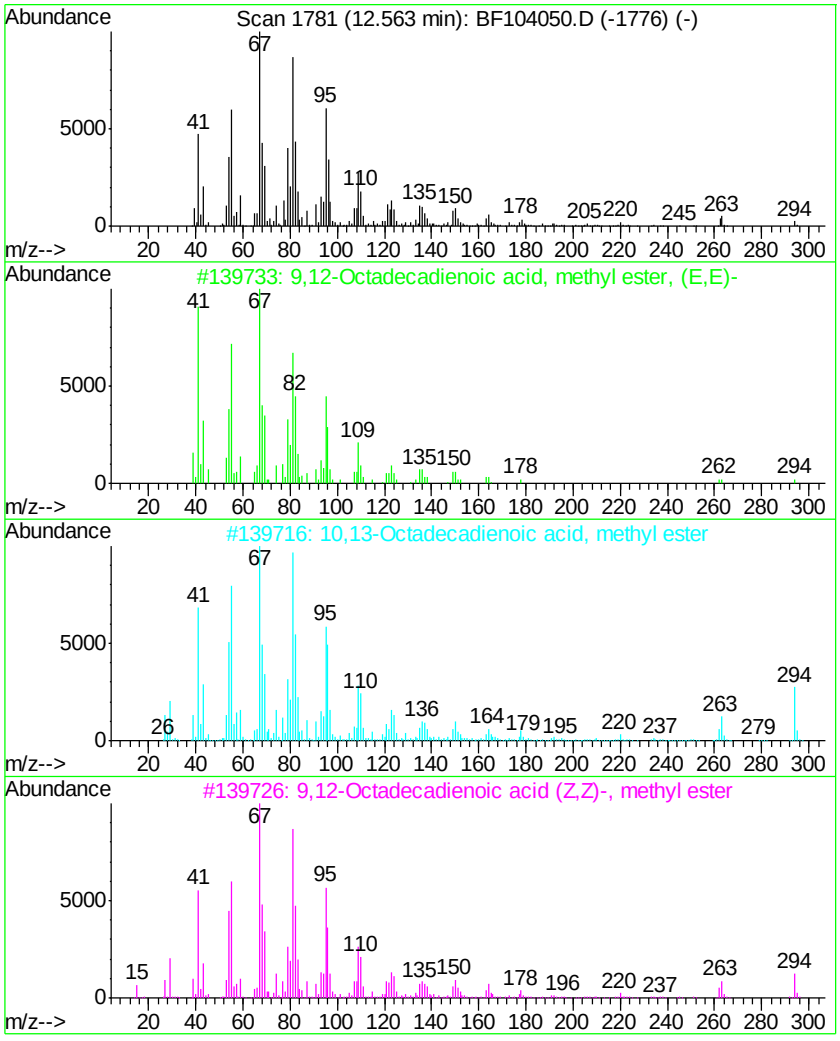
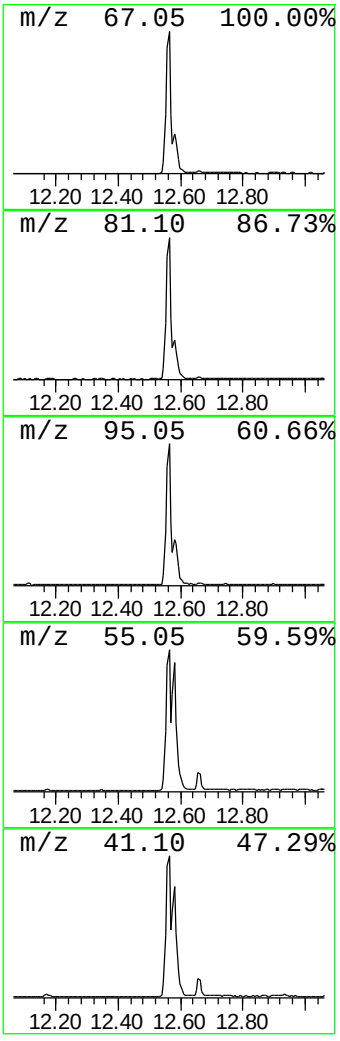
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	100.93 ng	3719110	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

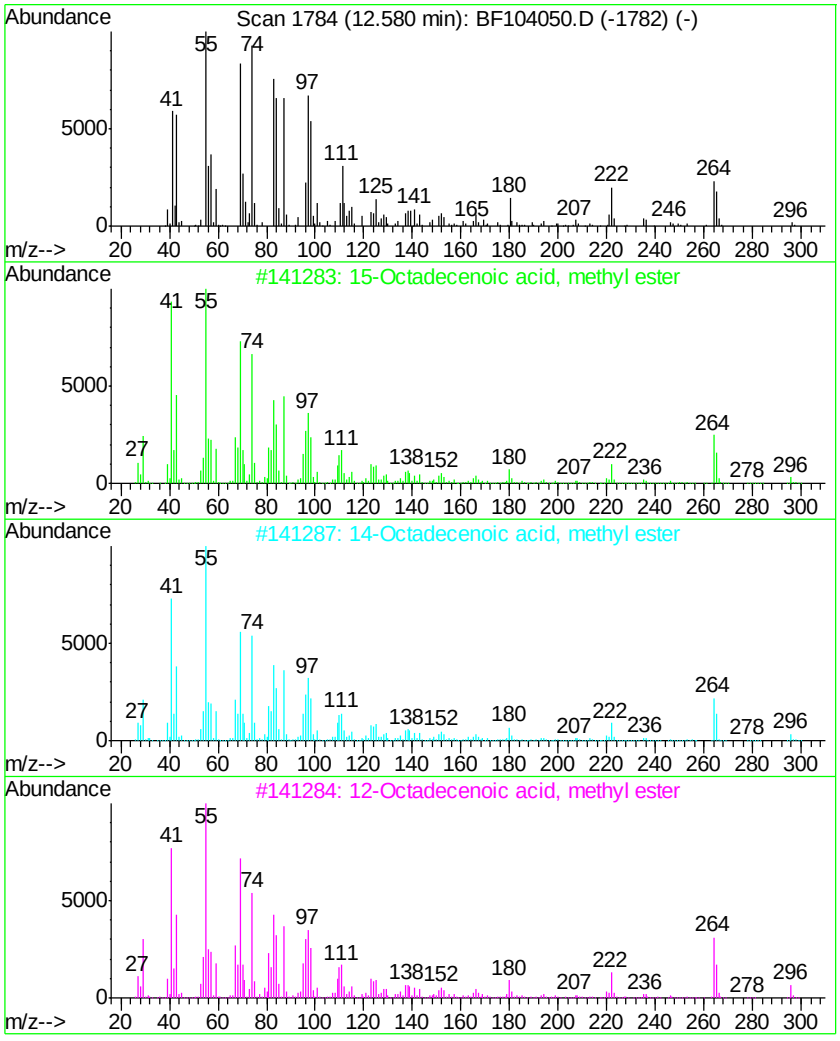
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

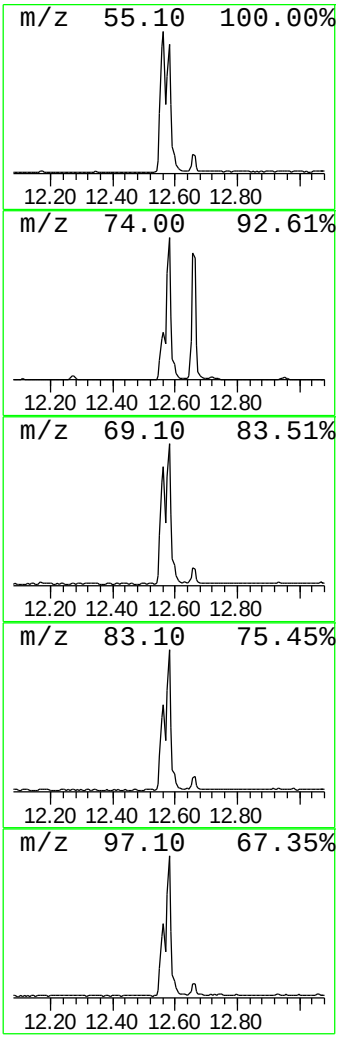
****

Peak Number 9 15-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	73.78 ng	2718630	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	90
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	89
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	89





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\
Data File : BF104050.D
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ALS Vial : 8 Sample Multiplier: 1

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
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TIC Library : C:\DATABASE\NIST11.L
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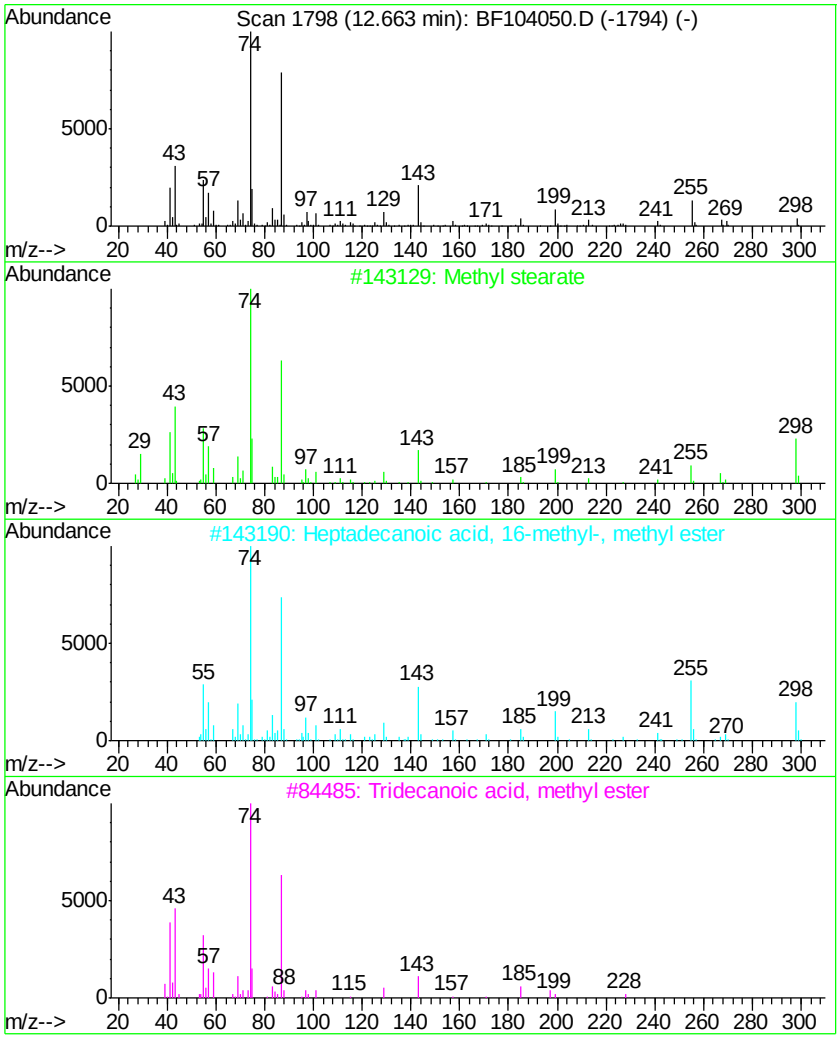
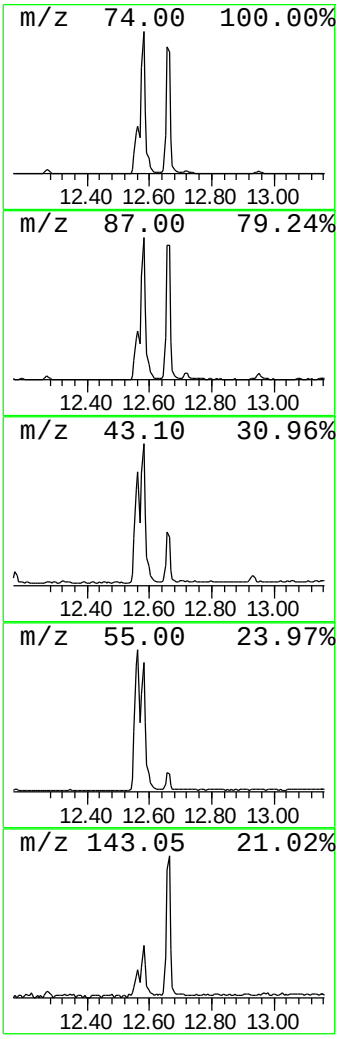
Peak Number 10 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	13.72 ng	505581	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032918\
Data File : BF104050.D
Acq On : 29 Mar 2018 14:56
Operator : JU/SJ
Sample : J1756-13 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-032718-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.73	6.73	17.4	ng	581534	1	6.96	668389	20.0
Dimethyl phthalate	9.70	2.4	ng	109487	3	10.00	920428	20.0
Dodecane	10.41	2.5	ng	117302	3	10.00	920428	20.0
Heptadecane	10.89	4.0	ng	146165	4	11.50	736997	20.0
Hexadecanoic acid...	11.87	31.0	ng	1141820	4	11.50	736997	20.0
4H-Cyclopenta[def...	12.12	2.5	ng	91059	4	11.50	736997	20.0
9,12-Octadecadien...	12.56	100.9	ng	3719110	4	11.50	736997	20.0
15-Octadecenoic a...	12.58	73.8	ng	2718630	4	11.50	736997	20.0
Methyl stearate	12.66	13.7	ng	505581	4	11.50	736997	20.0