LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097792.D
Acq On : 17 Aug 2017 18:06
Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

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-BF081517.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	2.204	17	20	32	rVV	1007014	1294635	37.31%	6.564%
2	2.310	32	38	54	rVB	2416646	3370873	97.15%	17.091%
3	2.804	116	122	128	rVB2	74505	123577	3.56%	0.627%
4	4.310	374	378	384	rBV2	23239	38193	1.10%	0.194%
5	6.769	793	796	800	rBV	981945	854371	24.62%	4.332%
6	8.057	1010	1015	1018	rBV	1269850	1053976	30.38%	5.344%
7	9.527	1261	1265	1269	rBV	168057	134869	3.89%	0.684%
8	9.810	1307	1313	1317	rBV	1317374	1072092	30.90%	5.436%
9	10.245	1384	1387	1390	rVB	54086	47416	1.37%	0.240%
10	10.721	1465	1468	1474	rBV	77953	96154	2.77%	0.488%
11	11.168	1541	1544	1546	rBV	66052	49950	1.44%	0.253%
12	11.292	1561	1565	1568	rBV	1206779	983026	28.33%	4.984%
13	11.598	1614	1617	1619	rBV	41283	36516	1.05%	0.185%
14	11.698	1630	1634	1637	rBV	1607566	1401572	40.39%	7.106%
15	12.004	1683	1686	1692	rVB4	38849	47445	1.37%	0.241%
16	12.386	1746	1751	1752	rBV	3684224	3469799	100.00%	17.592%
17	12.404	1752	1754	1761	rVV2	3187046	2989069	86.15%	15.155%
18	12.486	1765	1768	1773	rVB2	831467	717706	20.68%	3.639%
19	12.727	1806	1809	1813	rVB	75657	64187	1.85%	0.325%
20	13.121	1873	1876	1880	rBV3	44790	71880	2.07%	0.364%
21	13.209	1888	1891	1893	rBV	71254	69117	1.99%	0.350%
22	13.321	1907	1910	1914	rVB6	36180	41112	1.18%	0.208%
23	13.415	1924	1926	1931	rVB5	41745	41336	1.19%	0.210%
24	13.462	1931	1934	1938	rBV	39115	45047	1.30%	0.228%
25	13.786	1985	1989	1994	rBV4	66054	93587	2.70%	0.475%
26	13.880	2002	2005	2008	rBV	72988	63343	1.83%	0.321%
27	13.921	2008	2012	2016	rBV	846073	827488	23.85%	4.195%
28	15.356	2252	2256	2259	rVB	538480	624911	18.01%	3.168%

Sum of corrected areas: 19723247

LSC Report - Integrated Chromatogram

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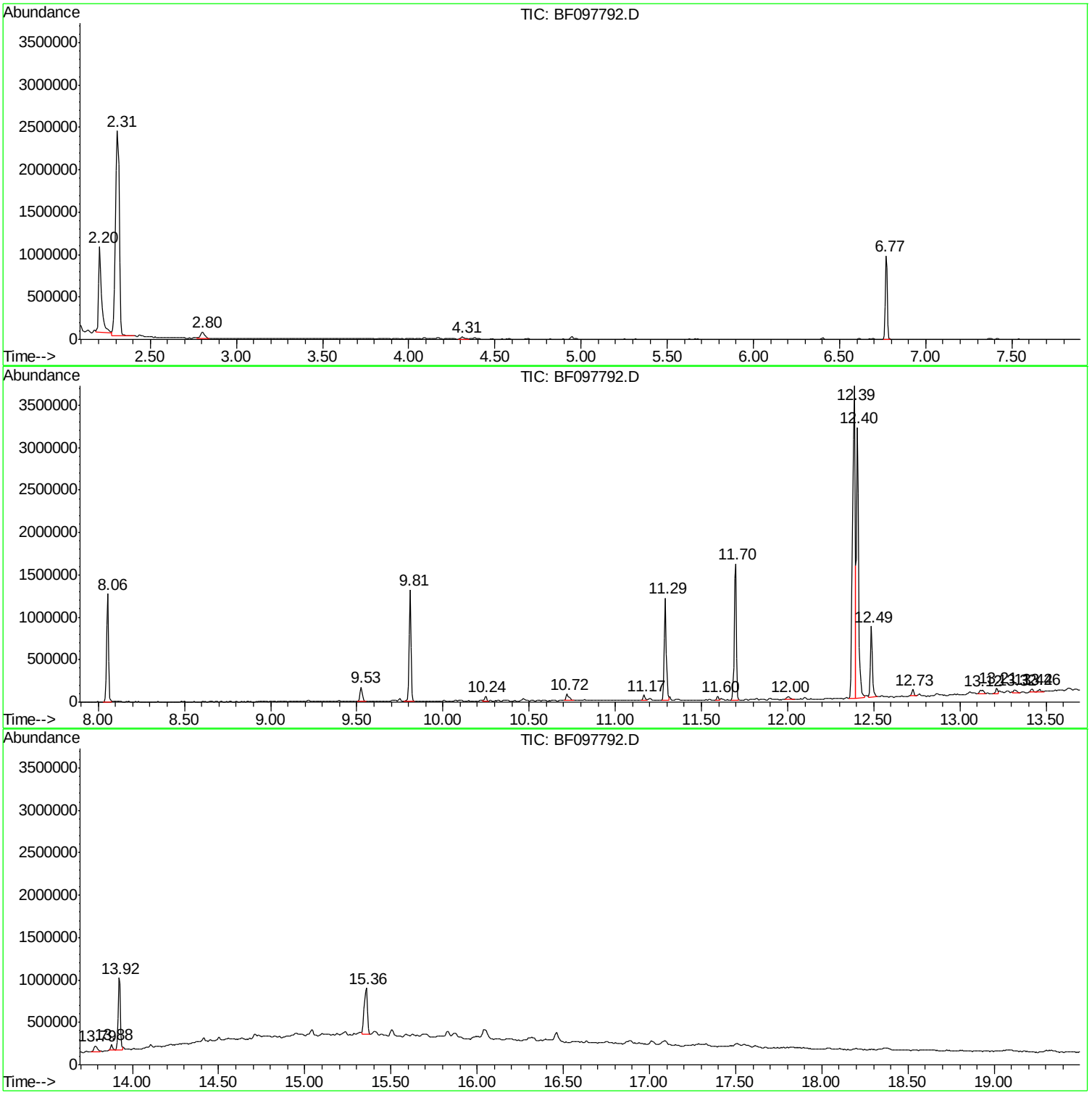
Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097792.D
Acq On : 17 Aug 2017 18:06
Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

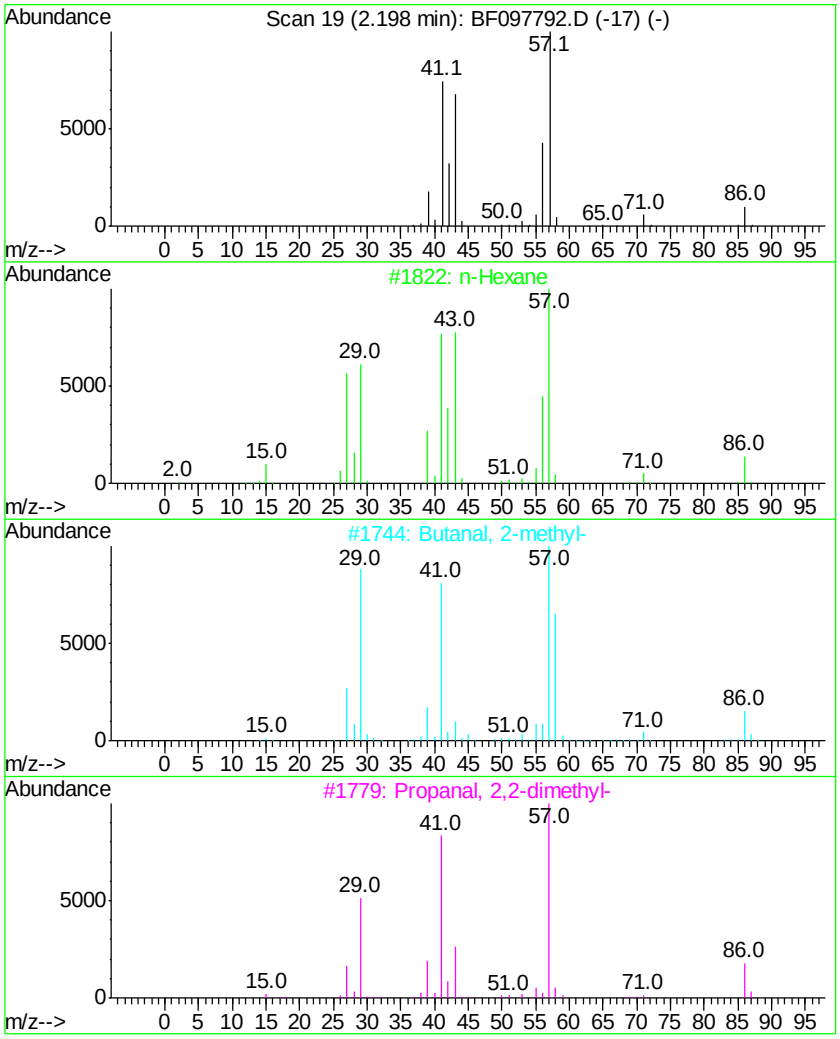
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

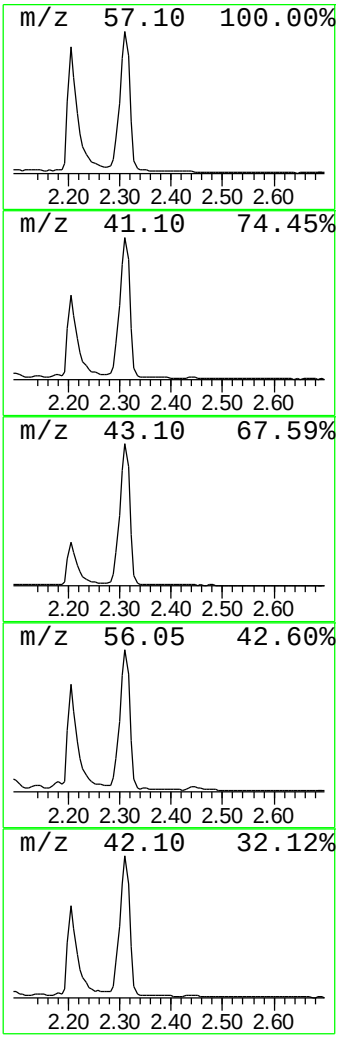
****

Peak Number 1 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	30.31 ng	1294640	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	28
5	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	28





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Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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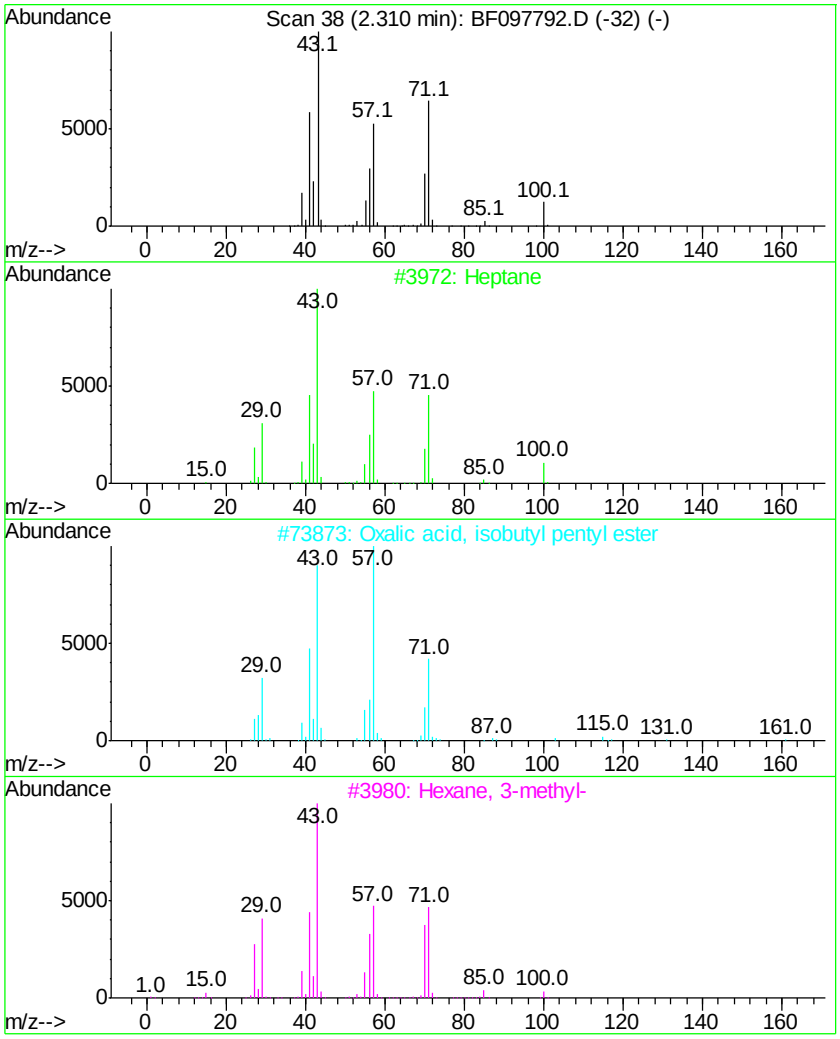
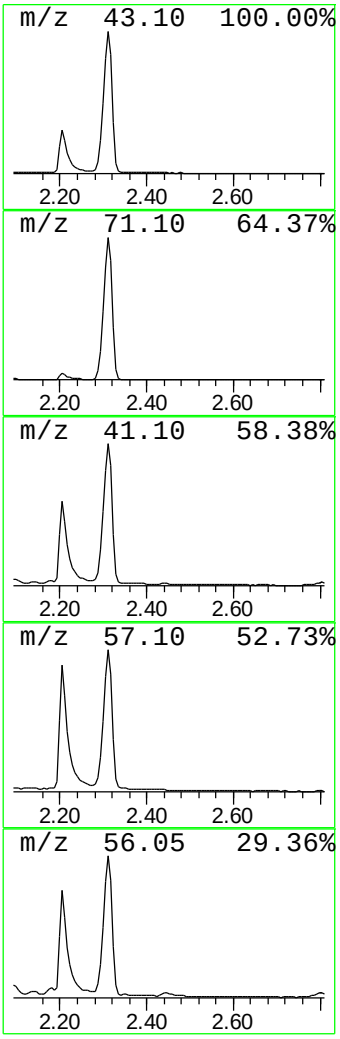
Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	78.91 ng	3370870	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	90
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	64
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	50
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	40
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097792.D
Acq On : 17 Aug 2017 18:06
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Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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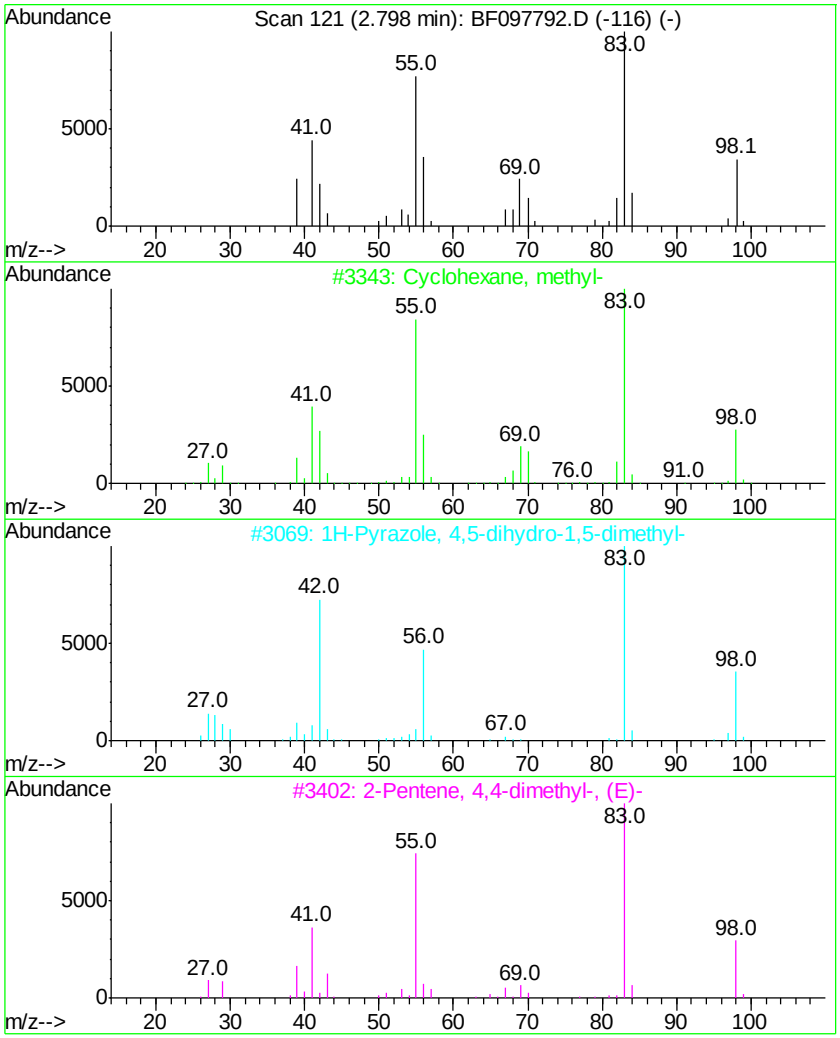
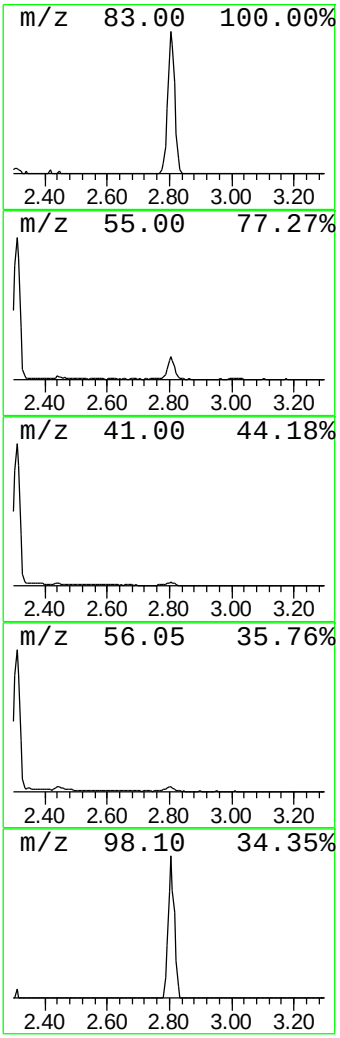
Peak Number 3 Cyclohexane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	2.89 ng	123577	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, methyl-	98	C7H14	000108-87-2	83
2	1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	59
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	58
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	58
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097792.D
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Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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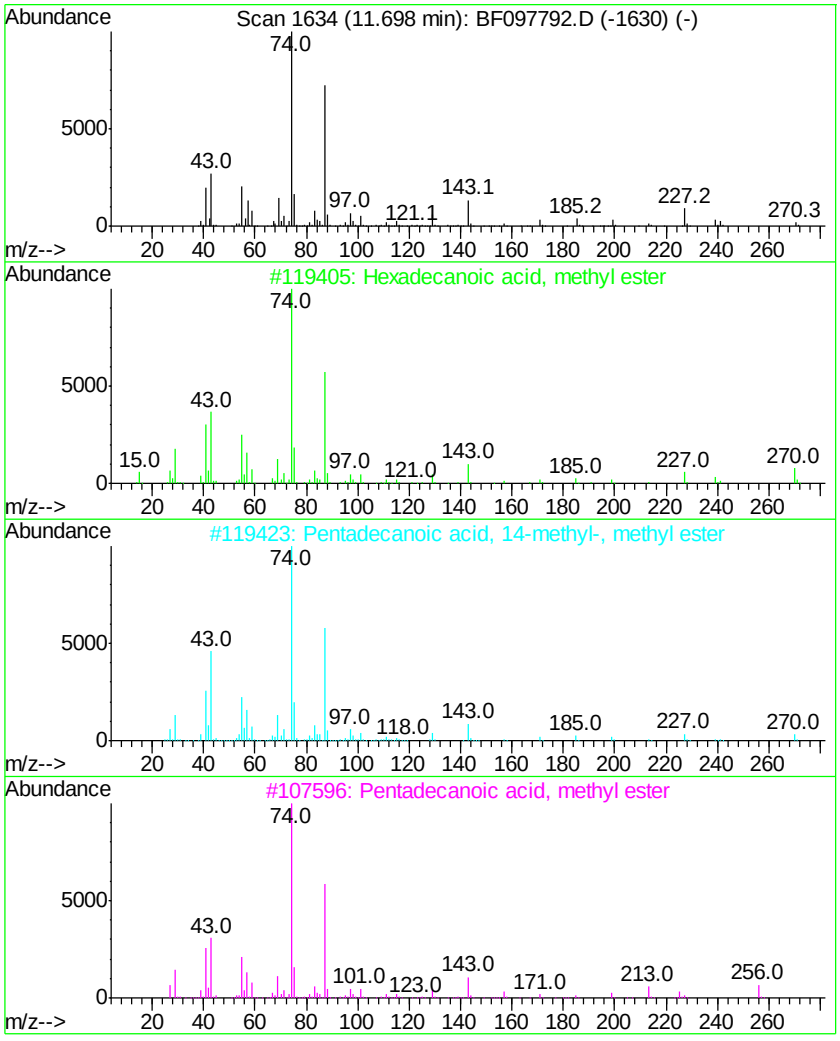
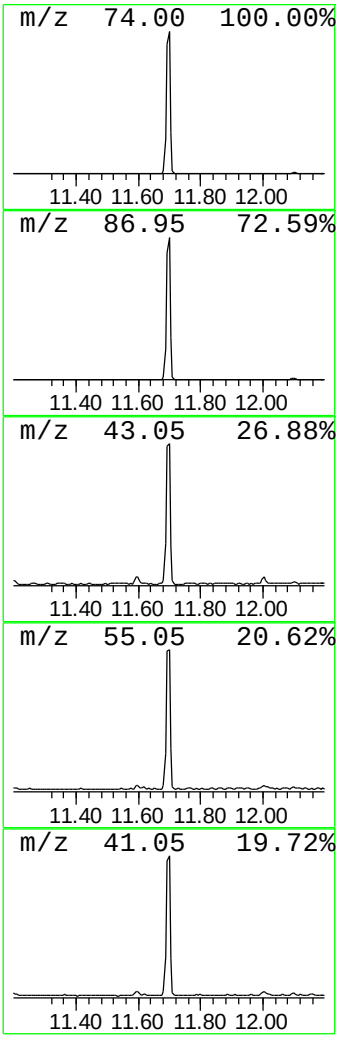
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	28.52 ng	1401570	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





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Operator : SJ/JU
Sample : I4798-04 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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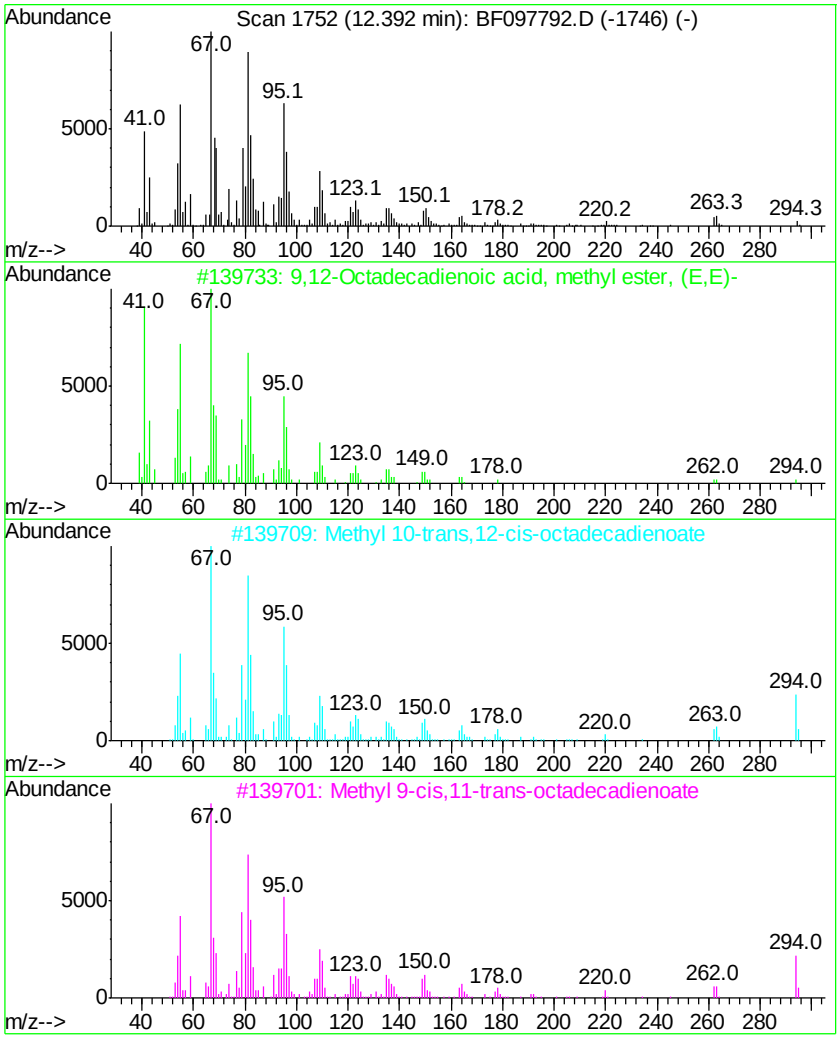
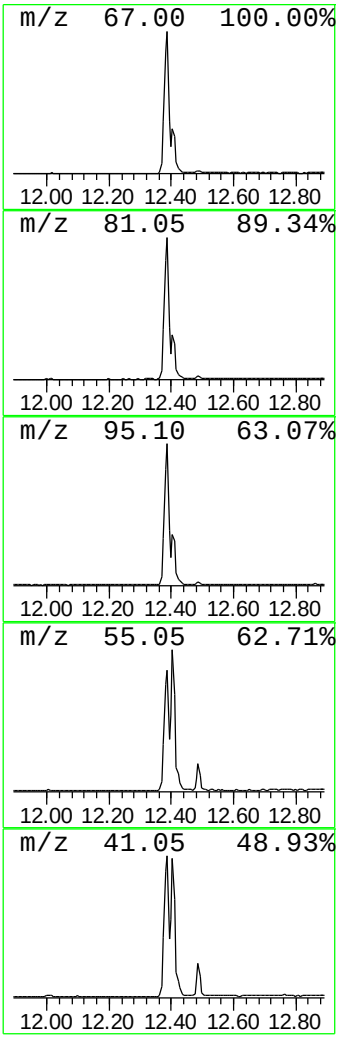
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	70.59 ng	3469800	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	96





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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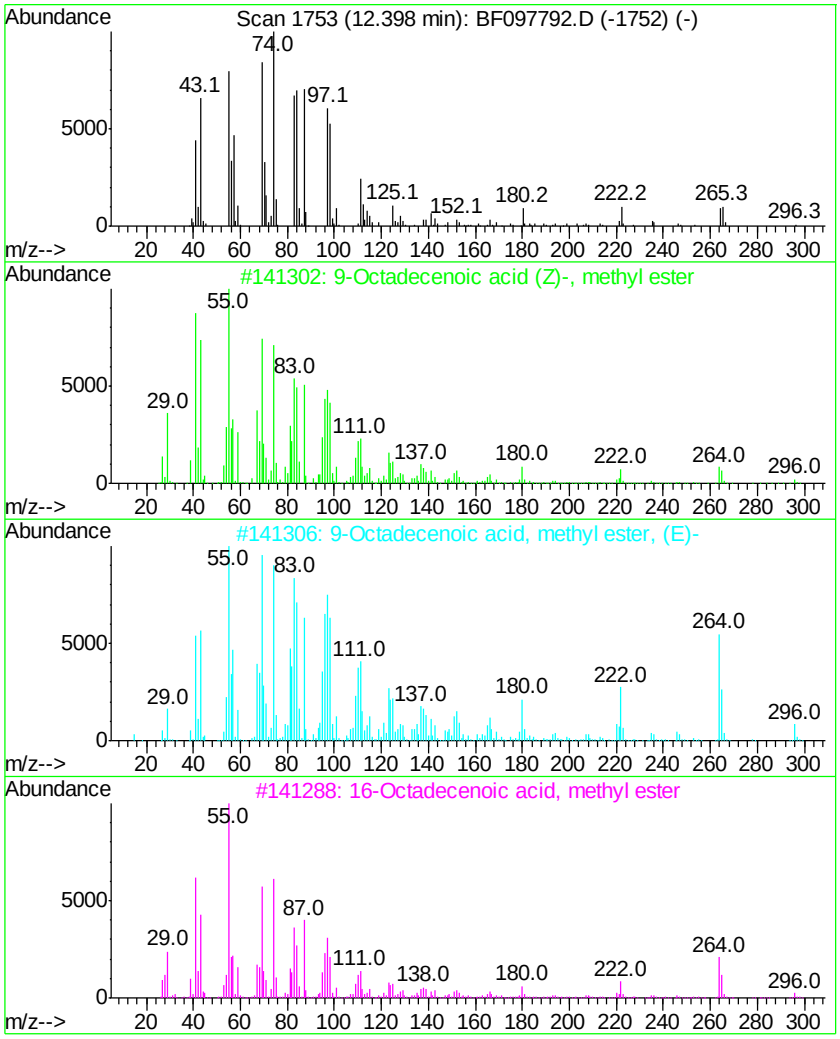
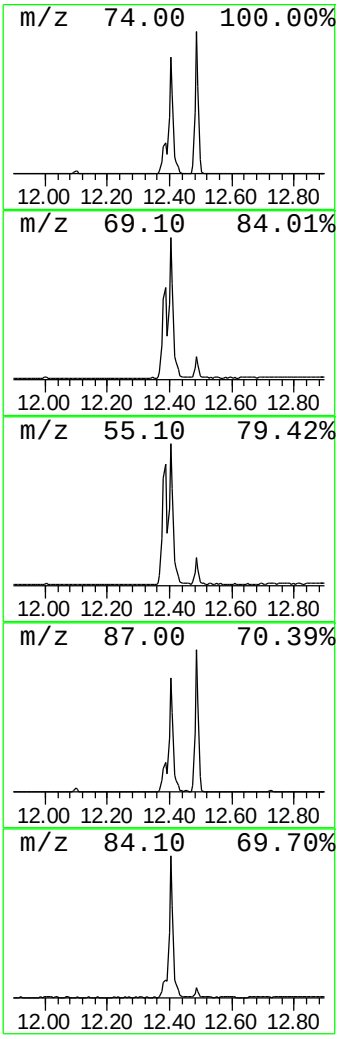
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	60.81 ng	2989070	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	83
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	52
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	46
5	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	46





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

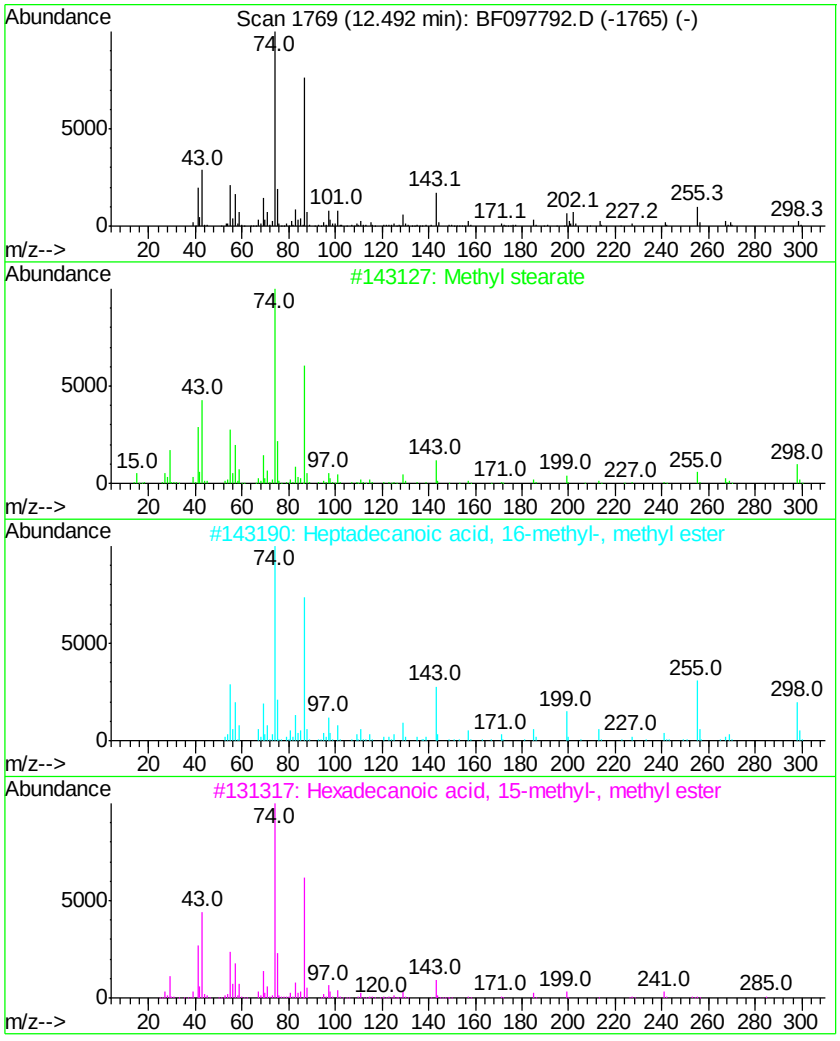
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

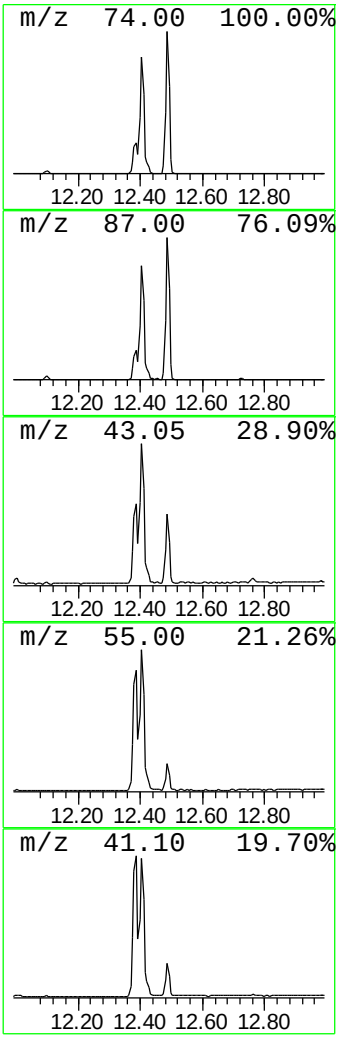
****

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	14.60 ng	717706	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91





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TIC Library : C:\DATABASE\NIST11.L
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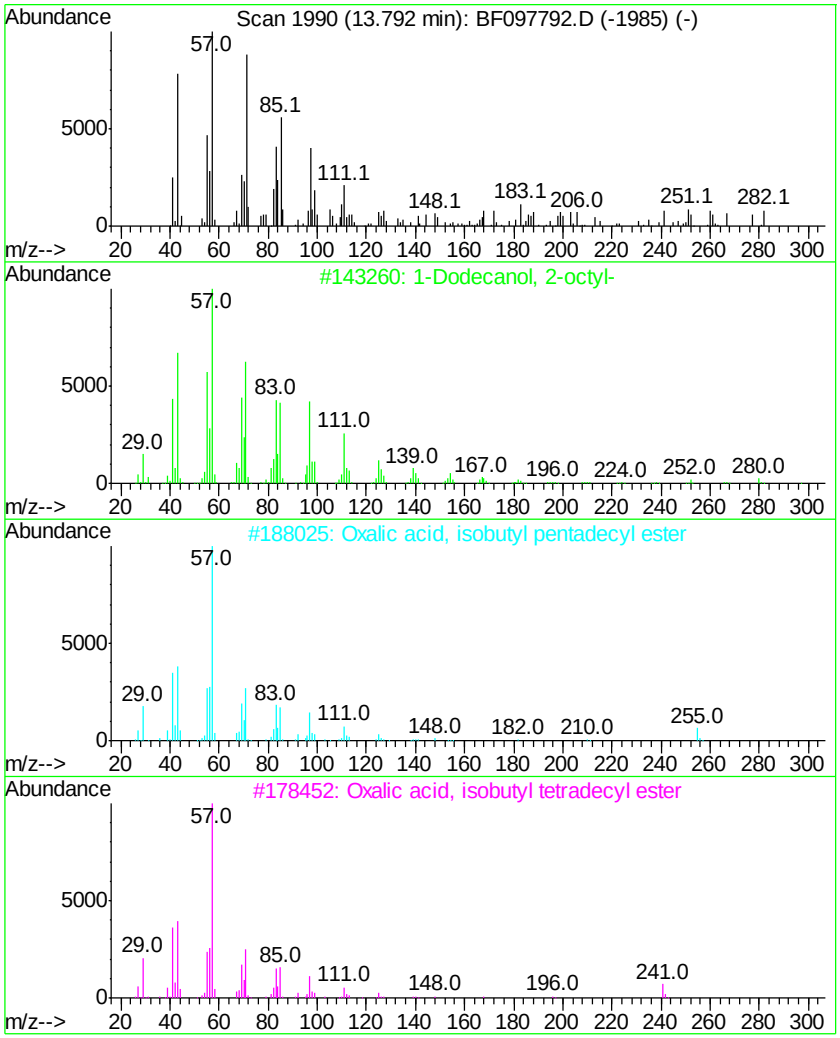
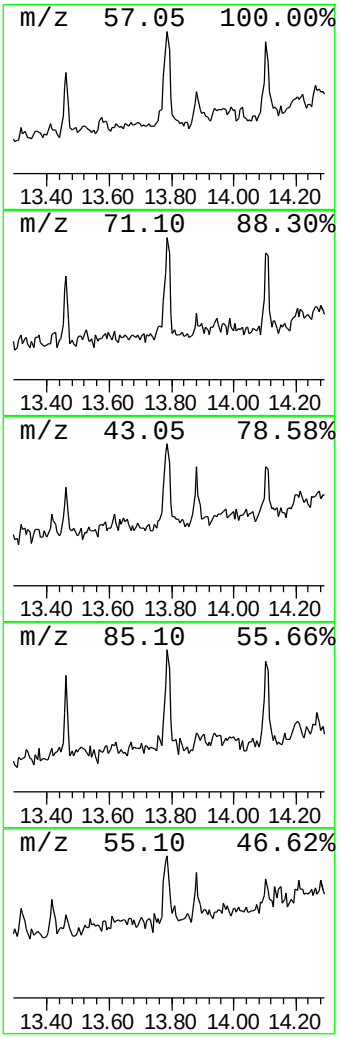
****

Peak Number 8 1-Dodecanol, 2-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.26 ng	93587	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
2	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	80
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	80
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	72
5	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
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Operator : SJ/JU
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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
n-Hexane	2.20	30.3	ng	1294640	1	6.77	854371	20.0
Heptane	2.31	78.9	ng	3370870	1	6.77	854371	20.0
Cyclohexane, methyl-	2.80	2.9	ng	123577	1	6.77	854371	20.0
Hexadecanoic acid...	11.70	28.5	ng	1401570	4	11.29	983026	20.0
9,12-Octadecadien...	12.39	70.6	ng	3469800	4	11.29	983026	20.0
9-Octadecenoic ac...	12.40	60.8	ng	2989070	4	11.29	983026	20.0
Methyl stearate	12.49	14.6	ng	717706	4	11.29	983026	20.0
1-Dodecanol, 2-oc...	13.79	2.3	ng	93587	5	13.92	827488	20.0