LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097217.D
Acq On : 31 Jul 2017 19:33
Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

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-BF072517.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	2.263	58	64	74	rVB	128099	195226	6.88%	0.779%
2	3.898	339	342	349	rBV2	21180	36646	1.29%	0.146%
3	4.616	460	464	482	rVB	557069	787607	27.76%	3.143%
4	5.093	541	545	561	rBV	2402186	2571885	90.65%	10.264%
5	5.781	657	662	667	rBV	24327	36152	1.27%	0.144%
6	6.157	722	726	739	rBV	2588561	2837181	100.00%	11.323%
7	6.257	739	743	750	rVB	2732732	2663649	93.88%	10.630%
8	6.481	777	781	789	rVB	817457	730244	25.74%	2.914%
9	6.634	803	807	811	rBV	2070218	1951833	68.79%	7.790%
10	7.051	873	878	881	rBV	1884604	1791734	63.15%	7.151%
11	7.763	995	999	1007	rBV	1161699	982486	34.63%	3.921%
12	8.839	1178	1182	1186	rBV	2264848	2140832	75.46%	8.544%
13	9.239	1247	1250	1255	rVB	340395	273171	9.63%	1.090%
14	9.510	1292	1296	1299	rBV	954728	823270	29.02%	3.286%
15	9.751	1334	1337	1341	rBV3	37168	39963	1.41%	0.159%
16	9.963	1370	1373	1376	rVB	54366	40512	1.43%	0.162%
17	10.298	1426	1430	1436	rBV	1182013	1063456	37.48%	4.244%
18	10.433	1450	1453	1460	rVB	82461	91982	3.24%	0.367%
19	10.880	1525	1529	1532	rBV	67548	54708	1.93%	0.218%
20	10.986	1543	1547	1549	rBV	666362	605998	21.36%	2.418%
21	11.004	1549	1550	1554	rVV	184424	148650	5.24%	0.593%
22	11.063	1557	1560	1564	rVB	43301	44301	1.56%	0.177%
23	11.304	1598	1601	1607	rVB3	31604	35334	1.25%	0.141%
24	11.486	1626	1632	1634	rBV3	30142	34586	1.22%	0.138%
25	11.545	1639	1642	1648	rVV3	93547	120756	4.26%	0.482%
26	11.592	1648	1650	1653	rVB	34819	32475	1.14%	0.130%
27	12.192	1748	1752	1756	rVB	334010	303808	10.71%	1.212%
28	12.327	1771	1775	1780	rBV4	32950	50736	1.79%	0.202%
29	12.416	1785	1790	1793	rVV	316105	320707	11.30%	1.280%
30	12.469	1796	1799	1806	rVB2	27139	32927	1.16%	0.131%
31	12.569	1812	1816	1820	rVB	1432051	1306745	46.06%	5.215%
32	12.751	1840	1847	1851	rVB2	43963	74149	2.61%	0.296%
33	12.816	1855	1858	1861	rVV2	50361	57435	2.02%	0.229%
34	12.851	1861	1864	1872	rVB2	35506	50957	1.80%	0.203%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097217.D
Acq On : 31 Jul 2017 19:33
Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.257	1930	1933	1936	rBV	31616	30931	1.09%	0.123%
36	13.363	1948	1951	1954	rBV	36148	38440	1.35%	0.153%
37	13.492	1970	1973	1982	rVB3	110000	149730	5.28%	0.598%
38	13.610	1985	1993	1996	rBV2	699745	837435	29.52%	3.342%
39	13.633	1996	1997	2001	rVB	169497	127799	4.50%	0.510%
40	13.716	2007	2011	2013	rBV	34999	36673	1.29%	0.146%
41	13.998	2055	2059	2063	rBV3	36535	40945	1.44%	0.163%
42	14.374	2121	2123	2125	rBV2	38066	33022	1.16%	0.132%
43	14.468	2136	2139	2143	rBV4	37445	53161	1.87%	0.212%
44	14.604	2158	2162	2170	rVB	196597	331051	11.67%	1.321%
45	14.692	2174	2177	2180	rVB2	69356	62221	2.19%	0.248%
46	14.727	2180	2183	2187	rBV4	40271	53497	1.89%	0.214%
47	14.857	2202	2205	2210	rVB	104435	112143	3.95%	0.448%
48	14.910	2211	2214	2219	rBV	146260	147282	5.19%	0.588%
49	14.962	2219	2223	2226	rBV	456335	495513	17.46%	1.978%
50	15.368	2288	2292	2296	rBV	53620	67848	2.39%	0.271%
51	16.186	2427	2431	2437	rBV	60258	107106	3.78%	0.427%

Sum of corrected areas: 25056898

LSC Report - Integrated Chromatogram

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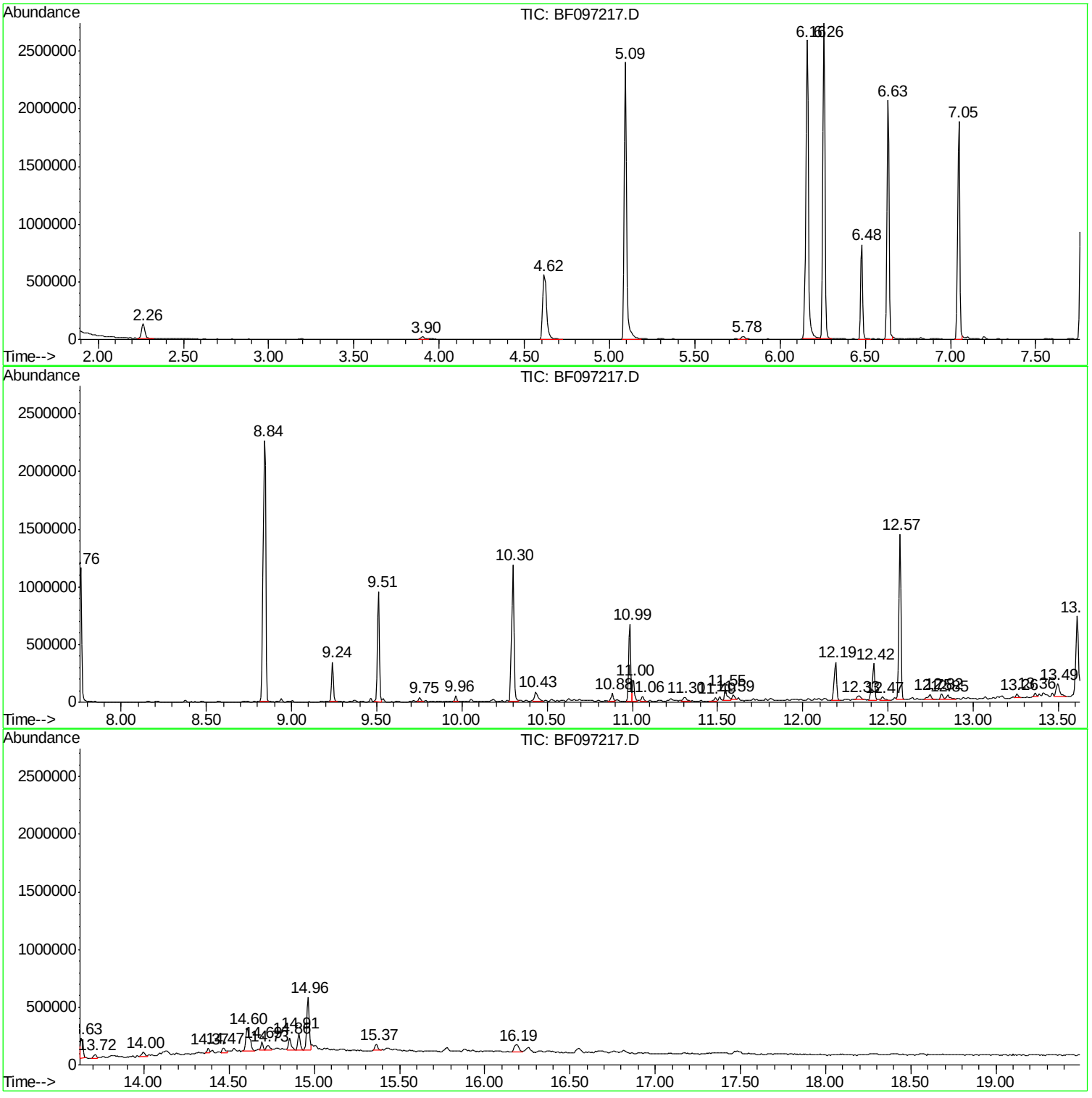
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF073117\
Data File : BF097217.D
Acq On : 31 Jul 2017 19:33
Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

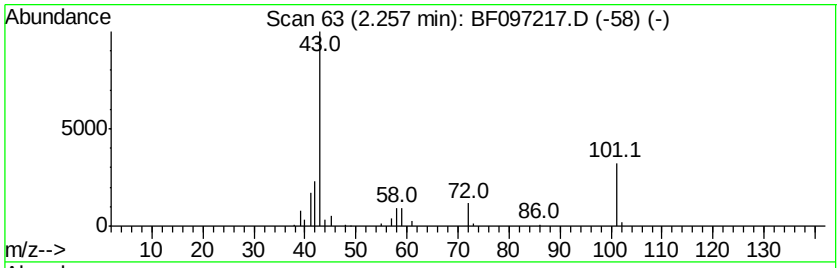
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

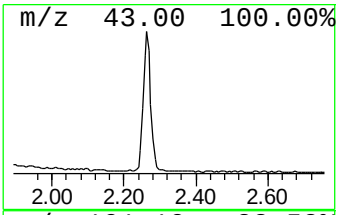
****

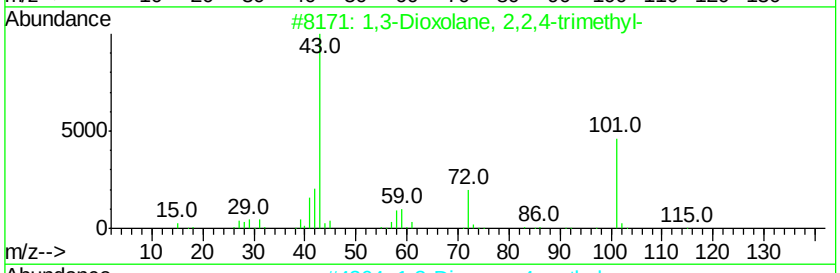
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 4

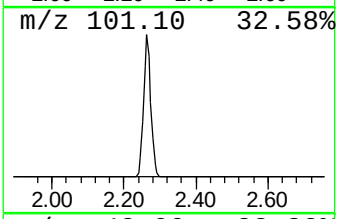
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	5.35 ng	195226	1,4-Dichlorobenzene-d4	6.48

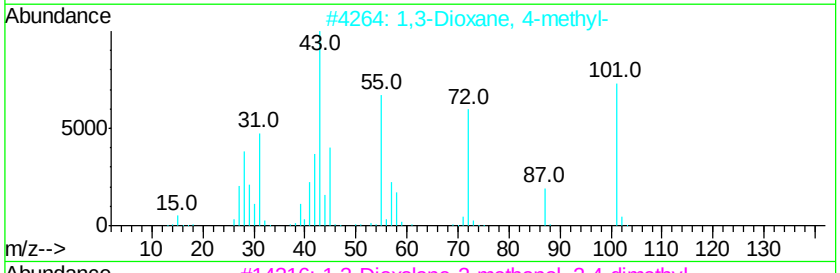
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	59
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	33
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	17
5	Isopropyl acetate	102	C5H10O2	000108-21-4	10

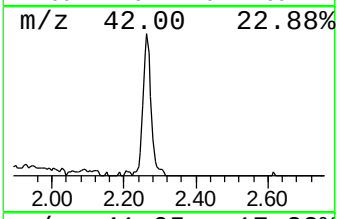


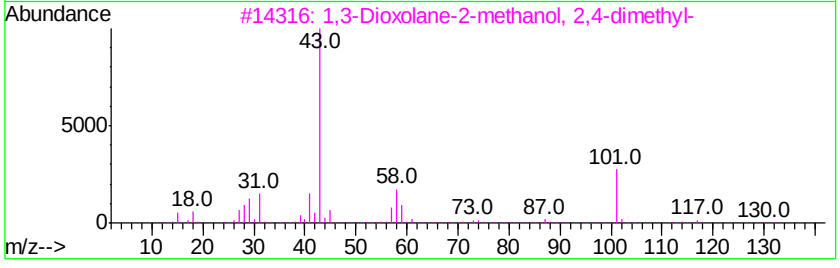


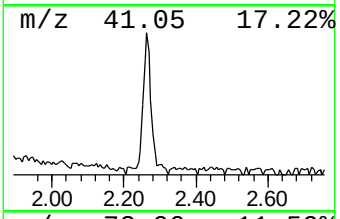


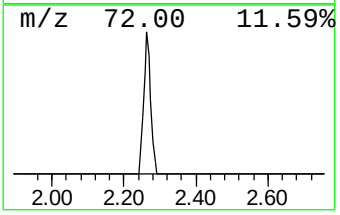












Library Search Compound Report

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Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

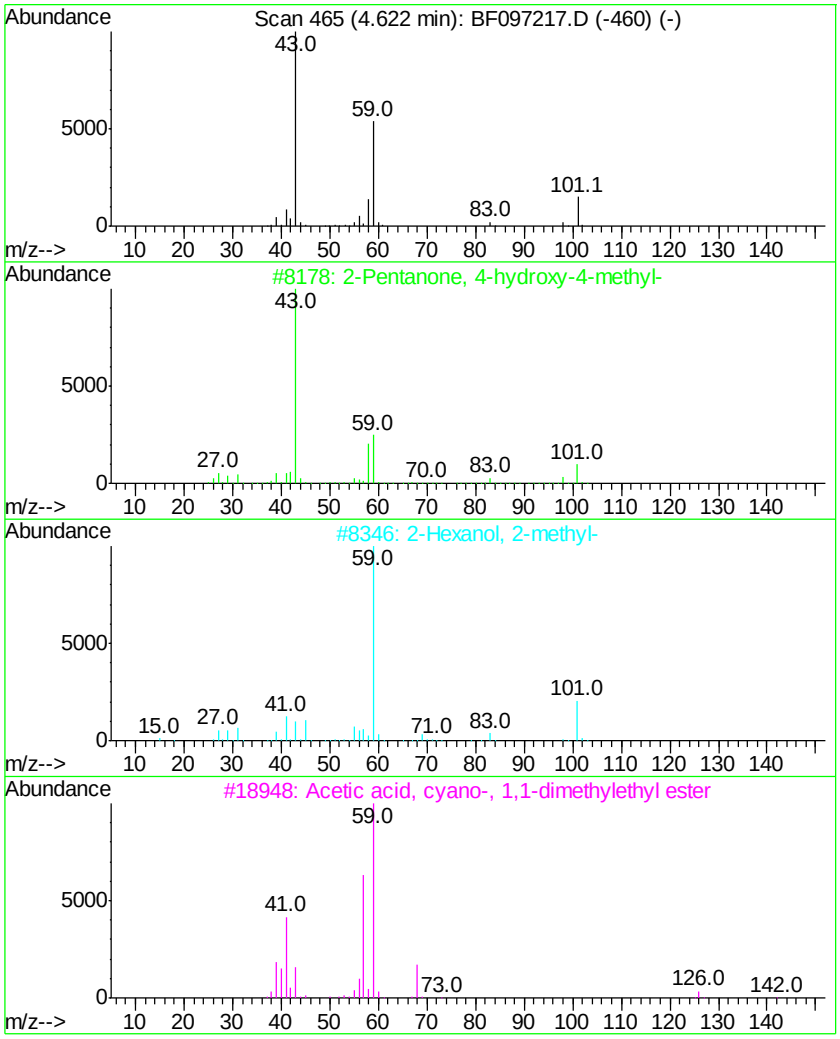
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

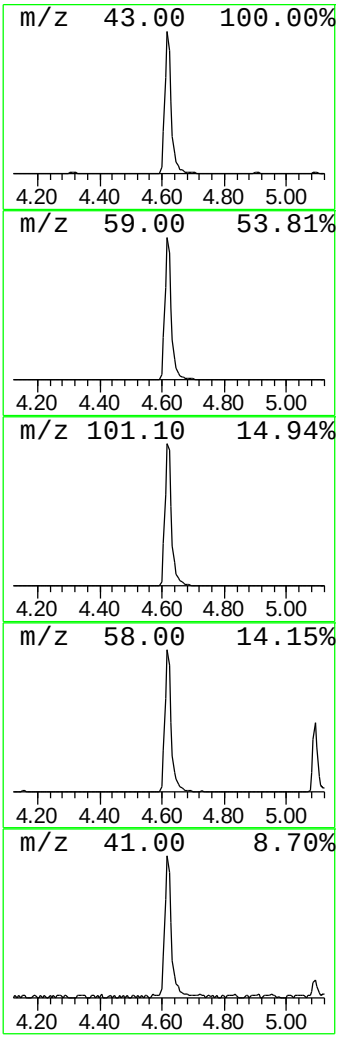
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	21.57 ng	787607	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	3-Hexanol	102	C6H14O	000623-37-0	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097217.D
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Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

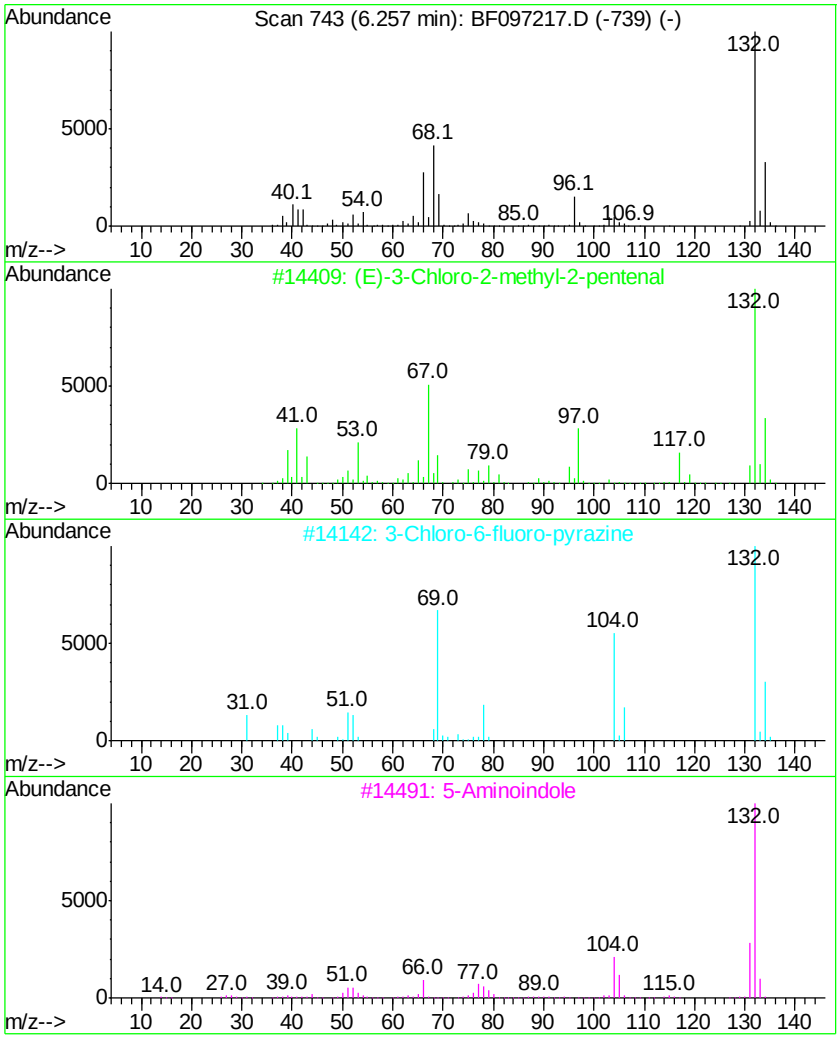
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

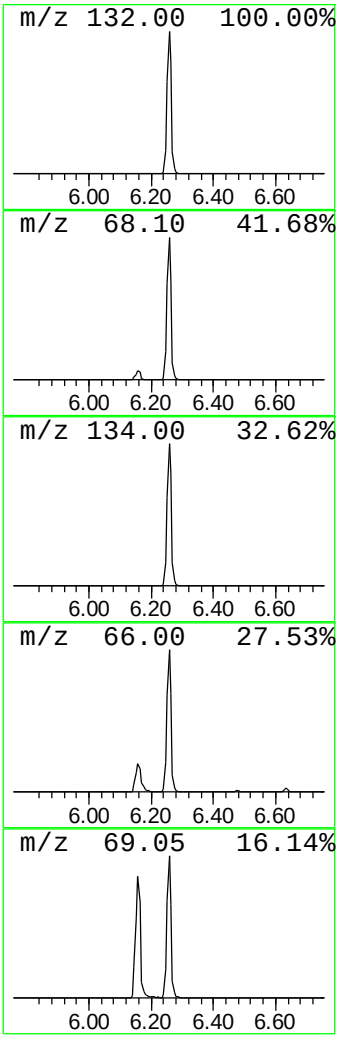
****

Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	72.95 ng	2663650	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

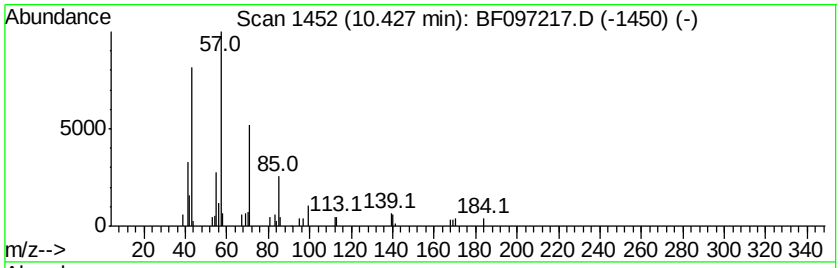
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

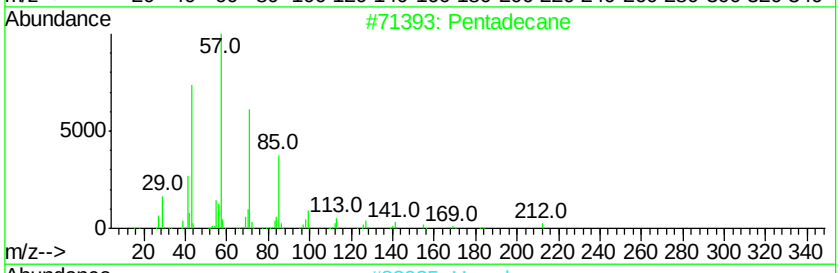
****

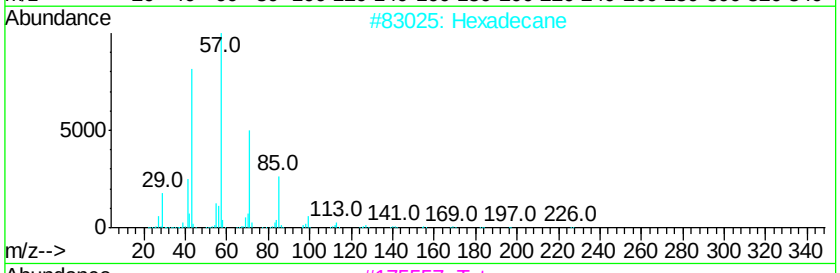
Peak Number 5 Pentadecane Concentration Rank 8

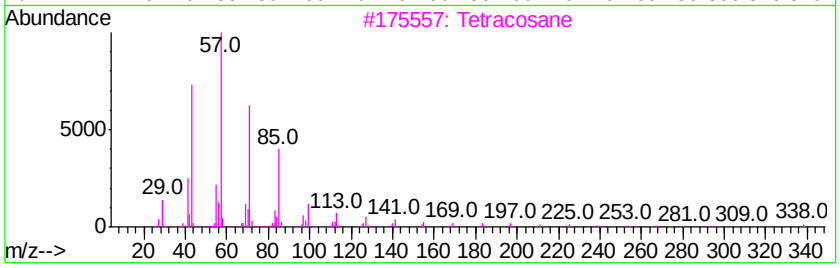
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	3.04 ng	91982	Phenanthrene-d10	10.99

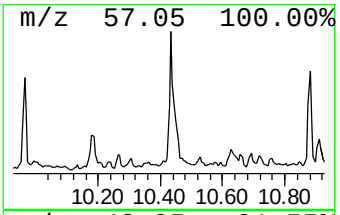
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Heptadecane	240	C17H36	000629-78-7	80

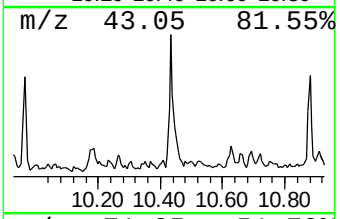


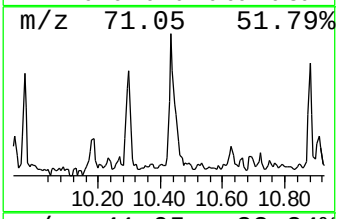


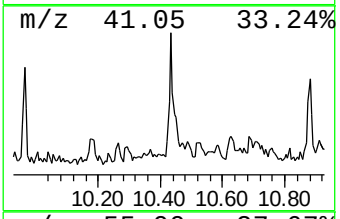


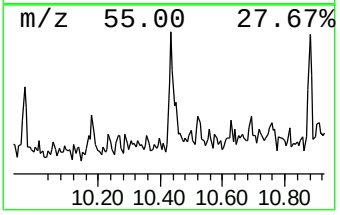












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

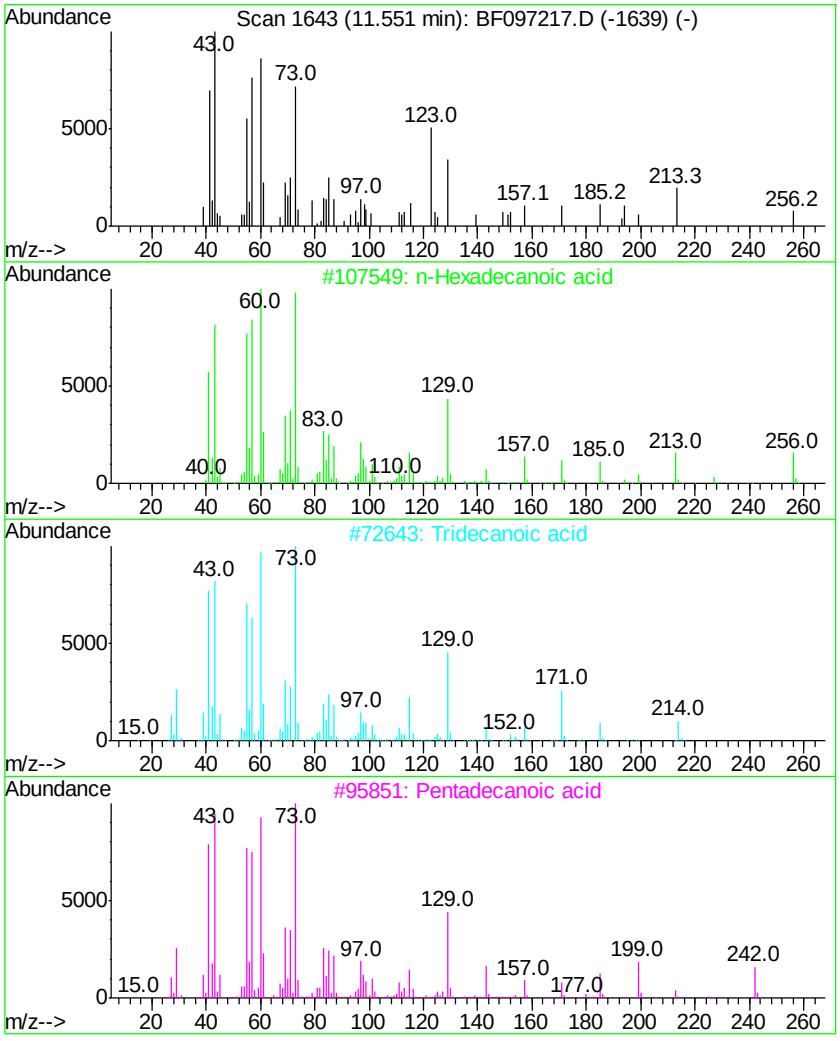
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

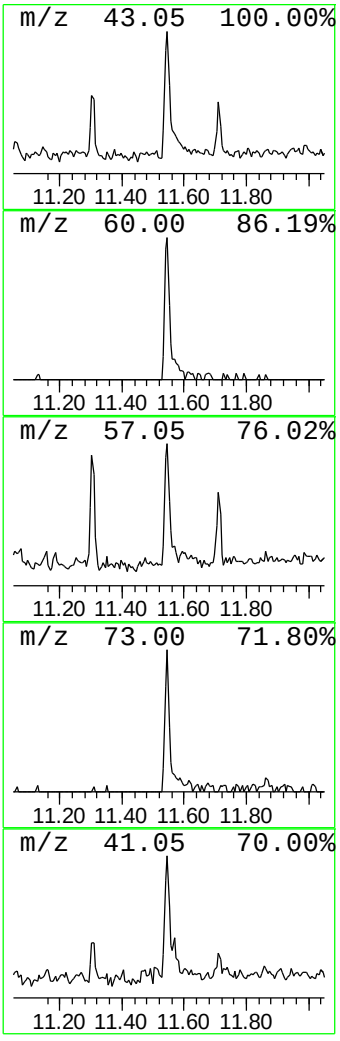
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	3.99 ng	120756	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	80





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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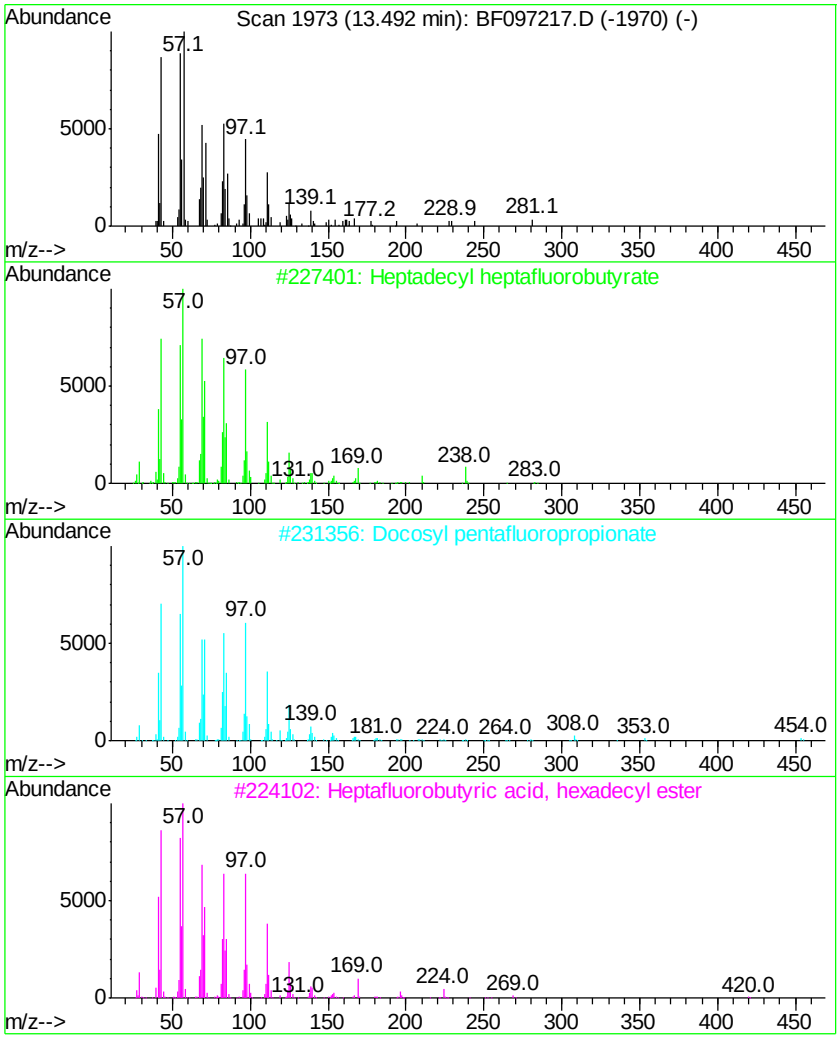
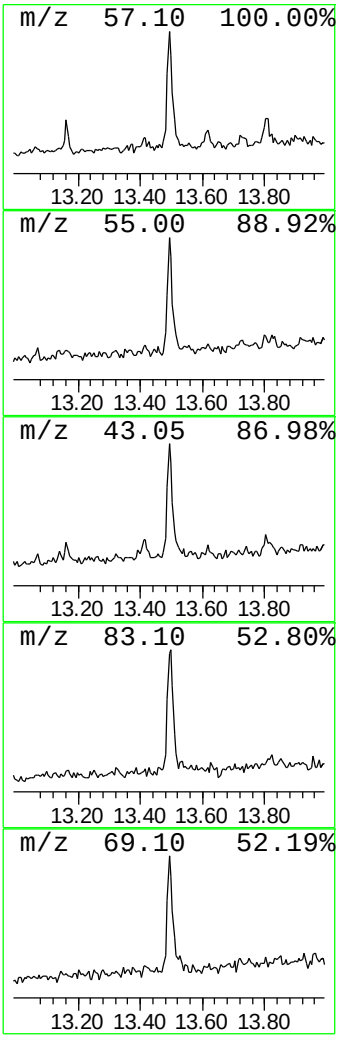
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.58 ng	149730	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097217.D
Acq On : 31 Jul 2017 19:33
Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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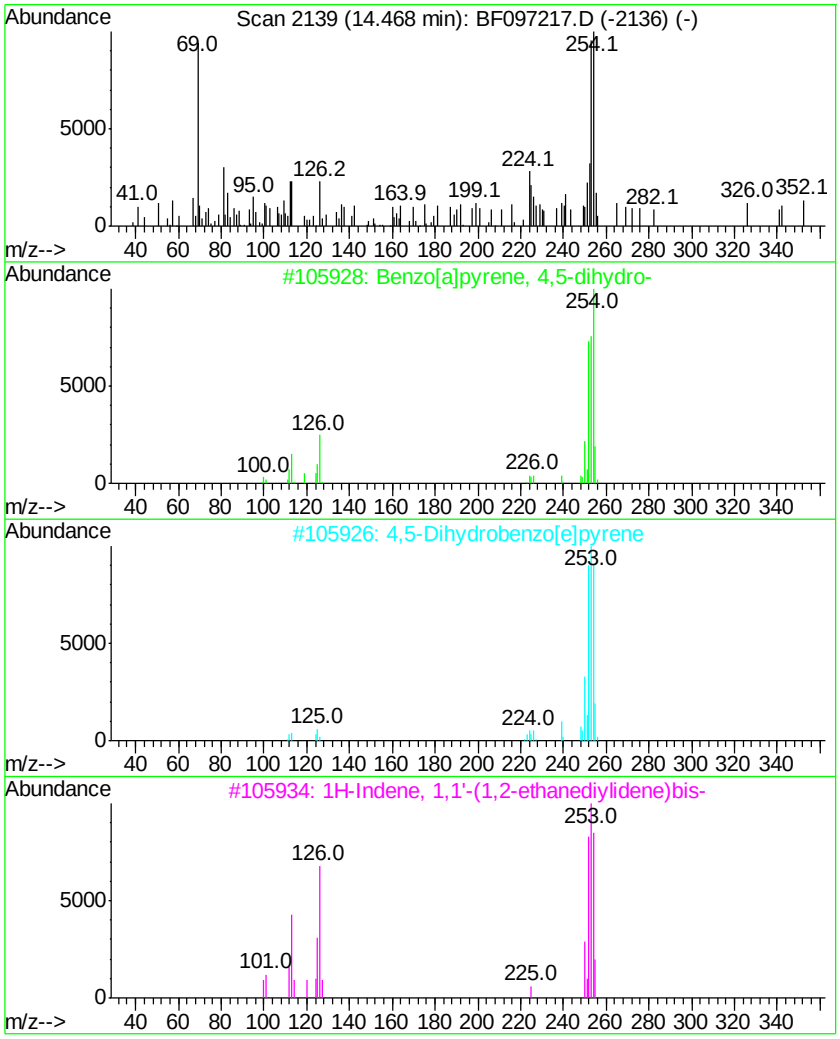
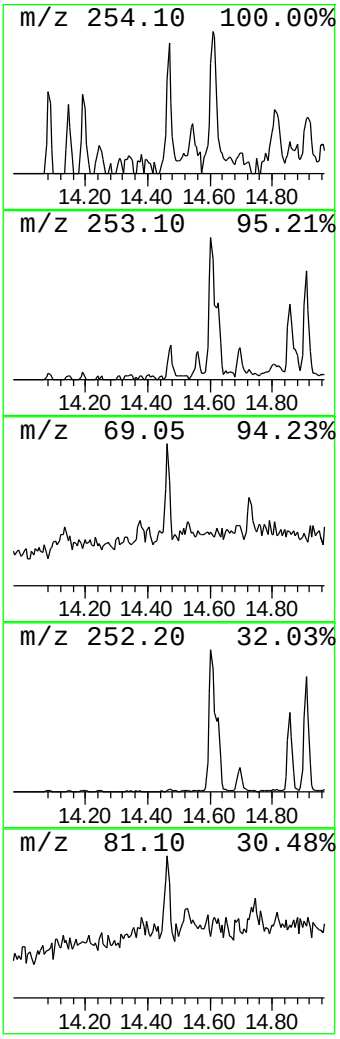
Peak Number 8 Benzo[a]pyrene, 4,5-dihydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.15 ng	53161	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene, 4,5-dihydro-	254	C20H14	057652-66-1	52
2	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	50
3	1H-Indene, 1,1'-(1,2-ethanedivli...	254	C20H14	072088-04-1	47
4	1,1'-Binaphthalene	254	C20H14	000604-53-5	46
5	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	43





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Acq On : 31 Jul 2017 19:33
Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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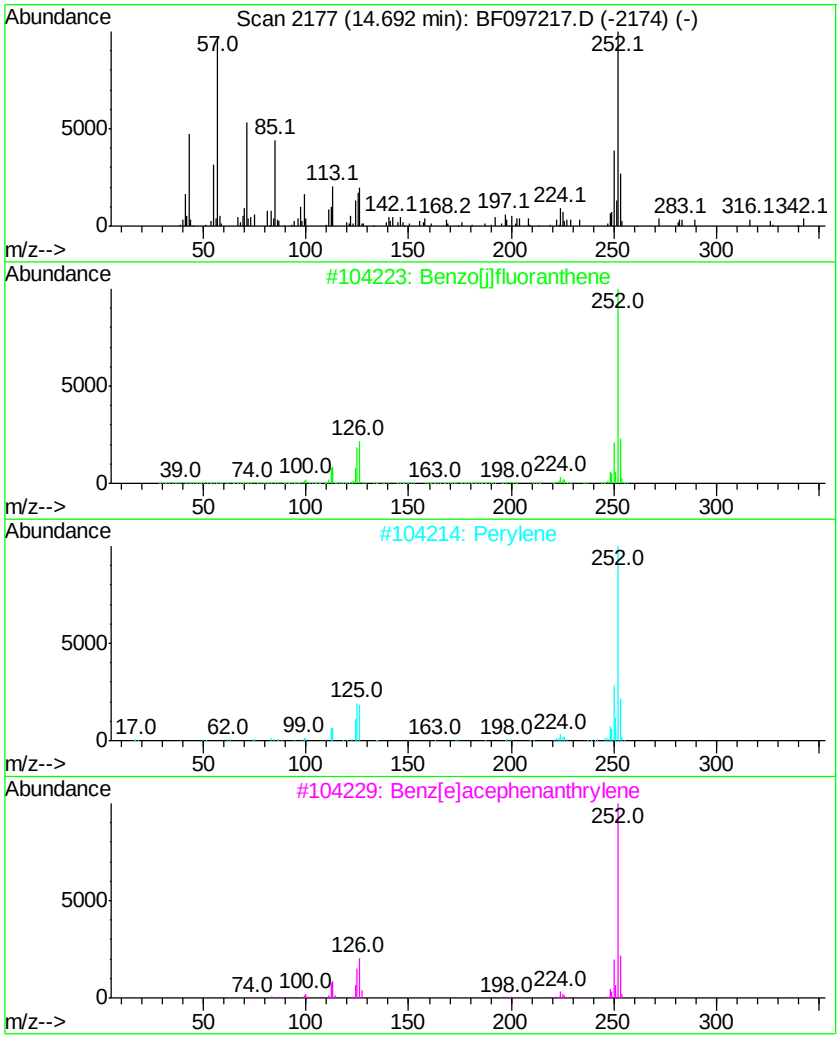
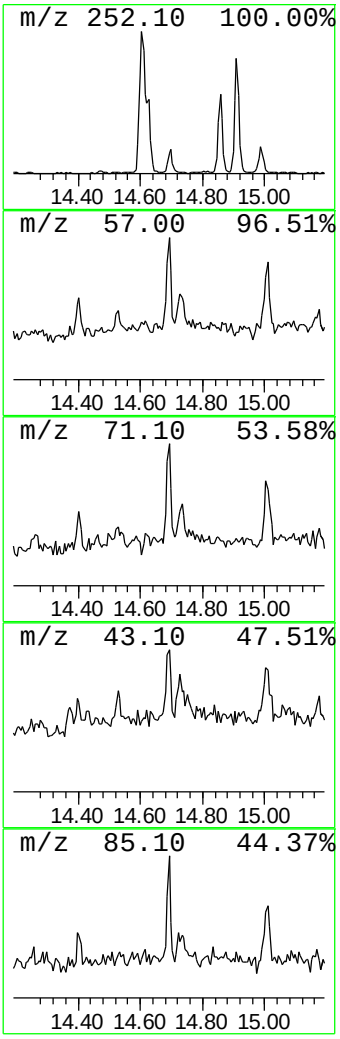
Peak Number 9 Benzo[j]fluoranthene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.51 ng	62221	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	83
2	Perylene	252	C20H12	000198-55-0	83
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
4	Benzo[a]pyrene	252	C20H12	000050-32-8	64
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	55





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Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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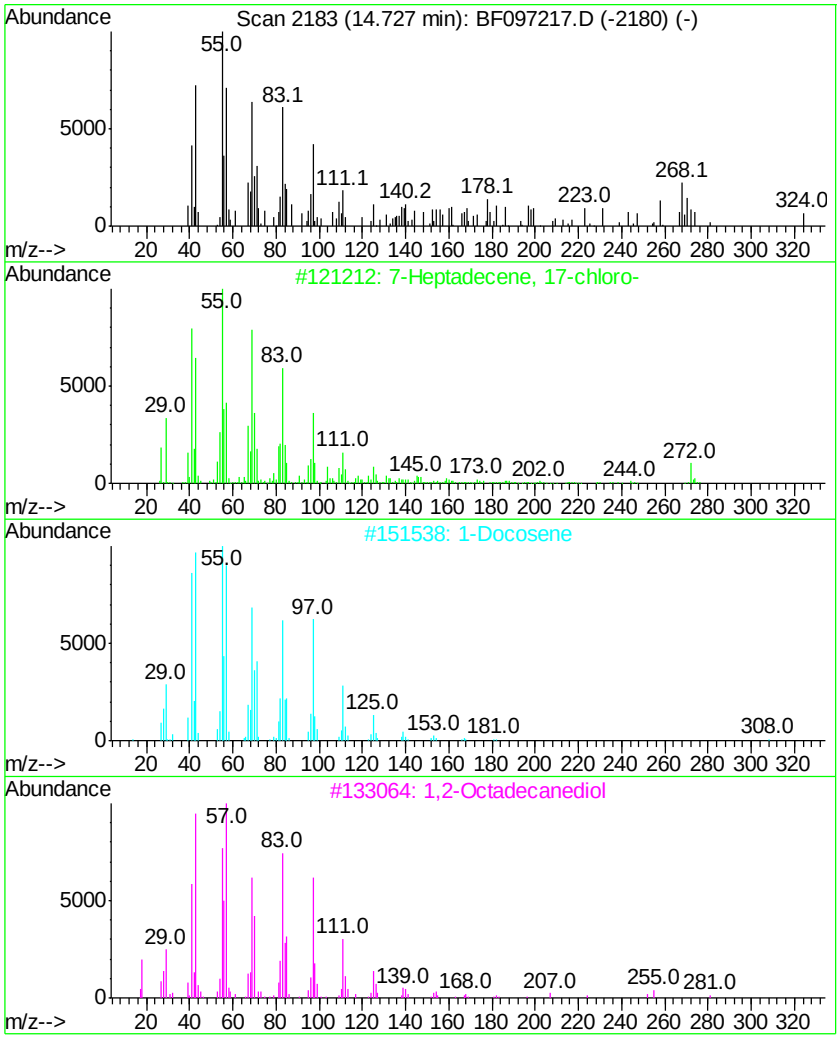
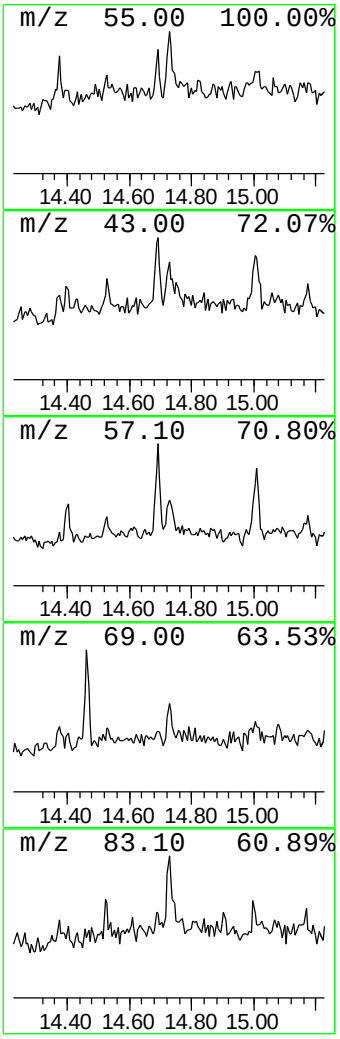
Peak Number 10 7-Heptadecene, 17-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.16 ng	53497	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	60
2	1-Docosene	308	C22H44	001599-67-3	53
3	1,2-Octadecanediol	286	C18H38O2	020294-76-2	52
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	52
5	Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	52





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Operator : SJ/JU
Sample : I4456-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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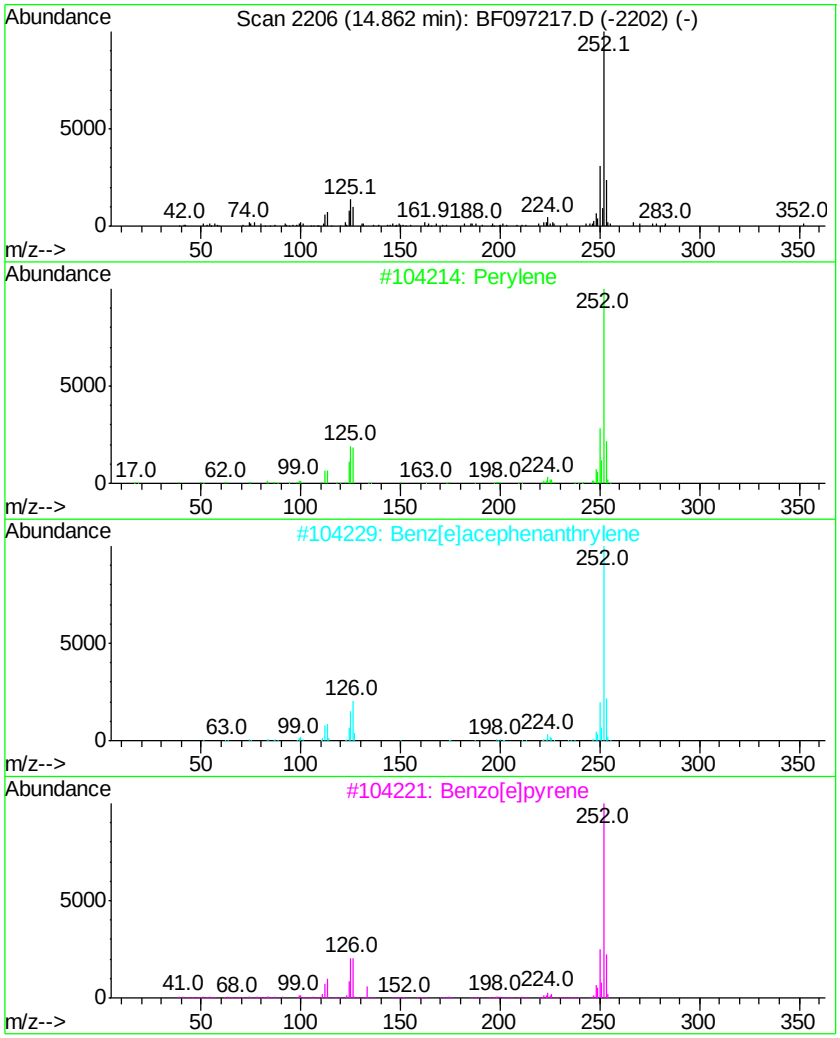
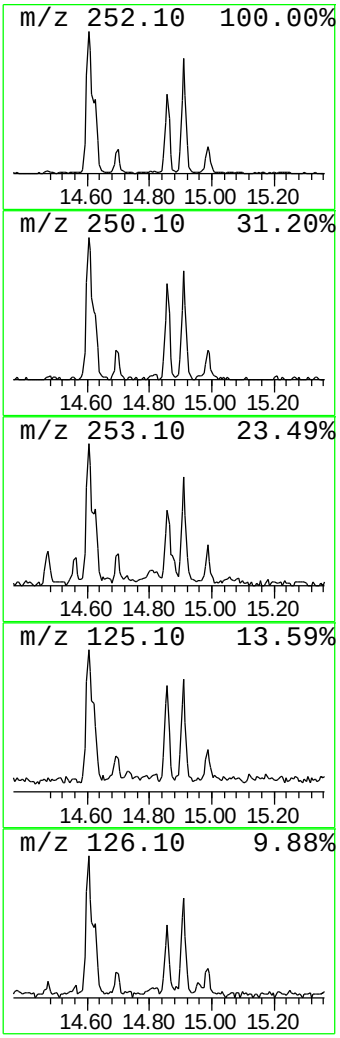
Peak Number 11 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	4.53 ng	112143	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96





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Sample : I4456-10
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-16-SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Integration Parameters: LSCINT.P

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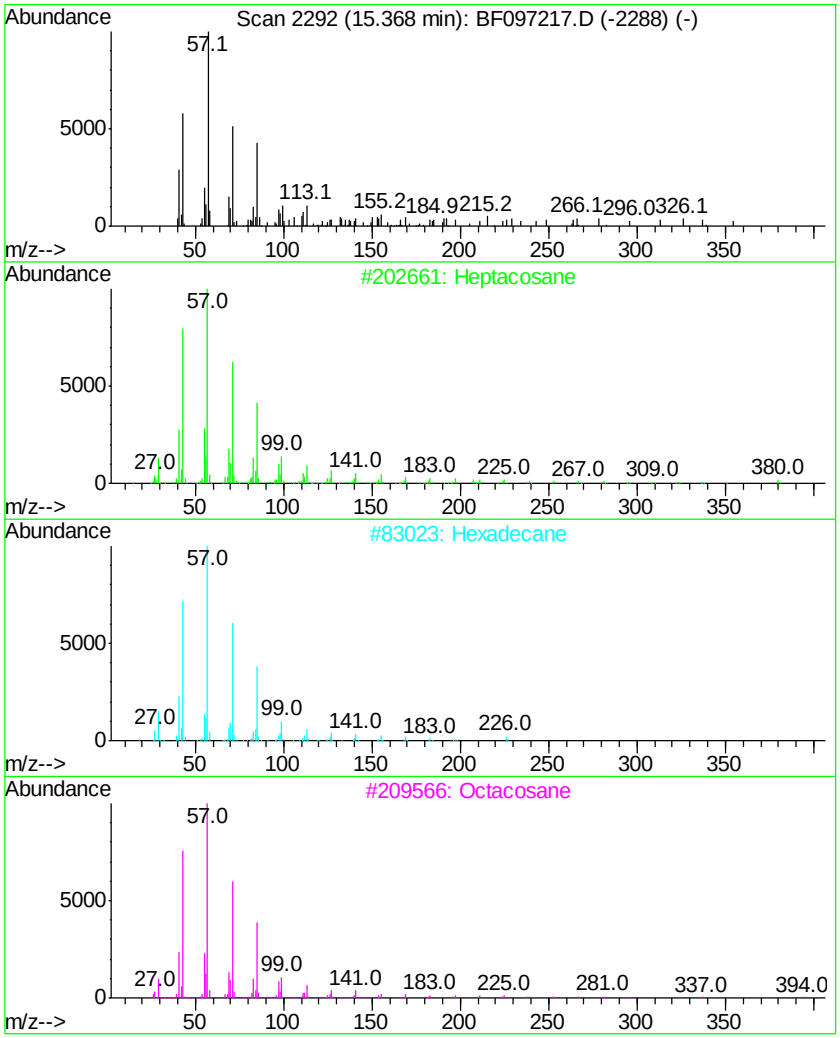
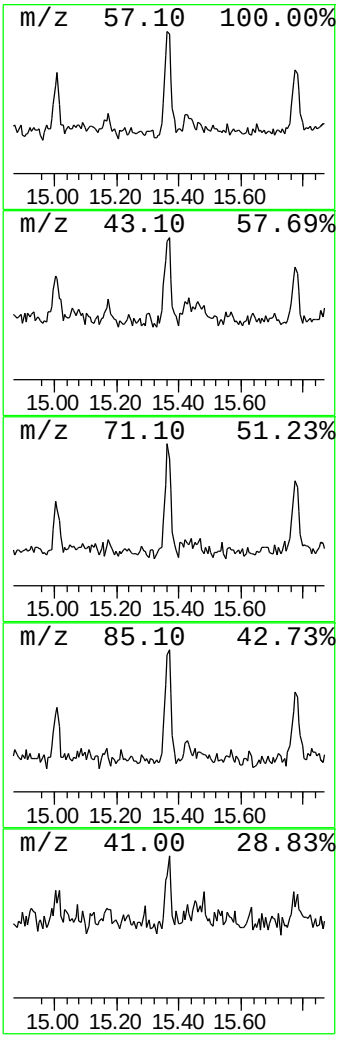
Peak Number 12 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.74 ng	67848	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Hexadecane	226	C16H34	000544-76-3	81
3	Octacosane	394	C28H58	000630-02-4	80
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Tentatively Identified Compound (LSC) summary

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ClientSampleId : TP-16-SS-7

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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
1,3-Dioxolane, 2,...	2.26	5.3	ng	195226	1	6.48	730244	20.0
2-Pentanone, 4-hy...	4.62	21.6	ng	787607	1	6.48	730244	20.0
unknown6.26	6.26	73.0	ng	2663650	1	6.48	730244	20.0
Pentadecane	10.43	3.0	ng	91982	4	10.99	605998	20.0
n-Hexadecanoic acid	11.55	4.0	ng	120756	4	10.99	605998	20.0
Heptadecyl heptaf...	13.49	3.6	ng	149730	5	13.61	837435	20.0
Benzo[a]pyrene, 4...	14.47	2.1	ng	53161	6	14.96	495513	20.0
Benzo[j]fluoranthene	14.69	2.5	ng	62221	6	14.96	495513	20.0
7-Heptadecene, 17...	14.73	2.2	ng	53497	6	14.96	495513	20.0
Perylene	14.86	4.5	ng	112143	6	14.96	495513	20.0
Heptacosane	15.37	2.7	ng	67848	6	14.96	495513	20.0