LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093871.D
Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-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-BF032217.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	2.110	34	38	46	rVB	117031	140643	3.03%	0.306%
2	4.140	378	383	392	rVB	619374	837033	18.01%	1.820%
3	4.516	441	447	450	rBV	4081022	4355190	93.72%	9.468%
4	4.910	509	514	518	rBV	54091	51780	1.11%	0.113%
5	5.569	619	626	631	rVB	3391368	4605064	99.10%	10.011%
6	5.728	647	653	656	rBV	4094801	4586333	98.69%	9.970%
7	5.987	693	697	701	rVB	1303432	1166479	25.10%	2.536%
8	6.169	722	728	731	rBV	3338433	3512170	75.58%	7.635%
9	6.634	800	807	810	rBV	2516537	2942956	63.33%	6.398%
10	7.486	947	952	956	rBV	1476134	1570189	33.79%	3.413%
11	8.816	1171	1178	1181	rBV	4315726	4646993	100.00%	10.102%
12	9.304	1256	1261	1265	rBV	444218	386068	8.31%	0.839%
13	9.457	1282	1287	1291	rVB	49747	57248	1.23%	0.124%
14	9.633	1308	1317	1321	rBV2	1628717	1679298	36.14%	3.651%
15	9.886	1356	1360	1364	rBV2	37423	50302	1.08%	0.109%
16	10.222	1413	1417	1420	rBV	103650	91242	1.96%	0.198%
17	10.304	1428	1431	1435	rVB	98059	92189	1.98%	0.200%
18	10.504	1457	1465	1472	rBV3	57218	98411	2.12%	0.214%
19	10.604	1476	1482	1485	rBV	2321442	2571380	55.33%	5.590%
20	10.810	1513	1517	1519	rBV	122968	137674	2.96%	0.299%
21	10.986	1541	1547	1550	rBV3	30034	47646	1.03%	0.104%
22	11.363	1608	1611	1615	rBV	112301	99517	2.14%	0.216%
23	11.457	1622	1627	1630	rBV2	1451716	1515940	32.62%	3.296%
24	11.486	1630	1632	1636	rVV	668577	552304	11.89%	1.201%
25	11.545	1636	1642	1646	rVB	182457	181410	3.90%	0.394%
26	11.892	1698	1701	1706	rVB	72715	74255	1.60%	0.161%
27	12.080	1729	1733	1736	rBV	117053	114753	2.47%	0.249%
28	12.110	1736	1738	1743	rVB	141895	145689	3.14%	0.317%
29	12.174	1743	1749	1752	rBV2	133933	155653	3.35%	0.338%
30	12.210	1752	1755	1758	rVV	178443	208194	4.48%	0.453%
31	12.239	1758	1760	1768	rVB	90840	96971	2.09%	0.211%
32	12.451	1792	1796	1801	rBV2	69101	99075	2.13%	0.215%
33	12.492	1801	1803	1808	rVB	61263	55473	1.19%	0.121%
34	12.763	1842	1849	1853	rBV	52187	84020	1.81%	0.183%

LSC Area Percent Report

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Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.945	1874	1880	1884	rBV	617663	600568	12.92%	1.306%
36	13.063	1896	1900	1903	rVB	72301	74891	1.61%	0.163%
37	13.221	1922	1927	1931	rVB	553345	591240	12.72%	1.285%
38	13.433	1957	1963	1967	rBV	2767239	3187054	68.58%	6.928%
39	13.510	1969	1976	1979	rBV4	39453	68938	1.48%	0.150%
40	13.615	1988	1994	1995	rBV4	39838	53814	1.16%	0.117%
41	13.639	1995	1998	2004	rVB	87215	92248	1.99%	0.201%
42	13.721	2008	2012	2015	rVV2	59512	60034	1.29%	0.131%
43	13.763	2016	2019	2030	rVB3	72523	104374	2.25%	0.227%
44	14.257	2097	2103	2110	rVB3	38968	59248	1.27%	0.129%
45	14.510	2143	2146	2153	rVB3	46387	62583	1.35%	0.136%
46	14.592	2156	2160	2170	rVV2	184137	287451	6.19%	0.625%
47	14.704	2174	2179	2183	rVV2	976983	1315291	28.30%	2.859%
48	14.733	2183	2184	2187	rVV	189901	167876	3.61%	0.365%
49	14.757	2187	2188	2194	rVB3	42004	52819	1.14%	0.115%
50	14.880	2203	2209	2216	rBV3	73993	109951	2.37%	0.239%
51	15.186	2256	2261	2265	rBV2	50054	61841	1.33%	0.134%
52	15.380	2292	2294	2300	rVB5	39992	49397	1.06%	0.107%
53	15.821	2365	2369	2373	rBV	140029	156548	3.37%	0.340%
54	15.927	2383	2387	2390	rBV	131219	194761	4.19%	0.423%
55	16.098	2413	2416	2420	rBV	58068	67647	1.46%	0.147%
56	16.221	2433	2437	2443	rVB	76314	84448	1.82%	0.184%
57	16.280	2443	2447	2452	rVB	125810	147136	3.17%	0.320%
58	16.345	2453	2458	2462	rBV	753076	932847	20.07%	2.028%
59	16.898	2547	2552	2555	rBV5	35158	54241	1.17%	0.118%
60	17.727	2688	2693	2702	rVB3	42402	91017	1.96%	0.198%
61	17.939	2718	2729	2735	rBV7	43202	122942	2.65%	0.267%
62	18.133	2758	2762	2769	rVB	35287	67956	1.46%	0.148%
63	18.345	2792	2798	2805	rVB8	30400	70800	1.52%	0.154%

Sum of corrected areas: 45999503

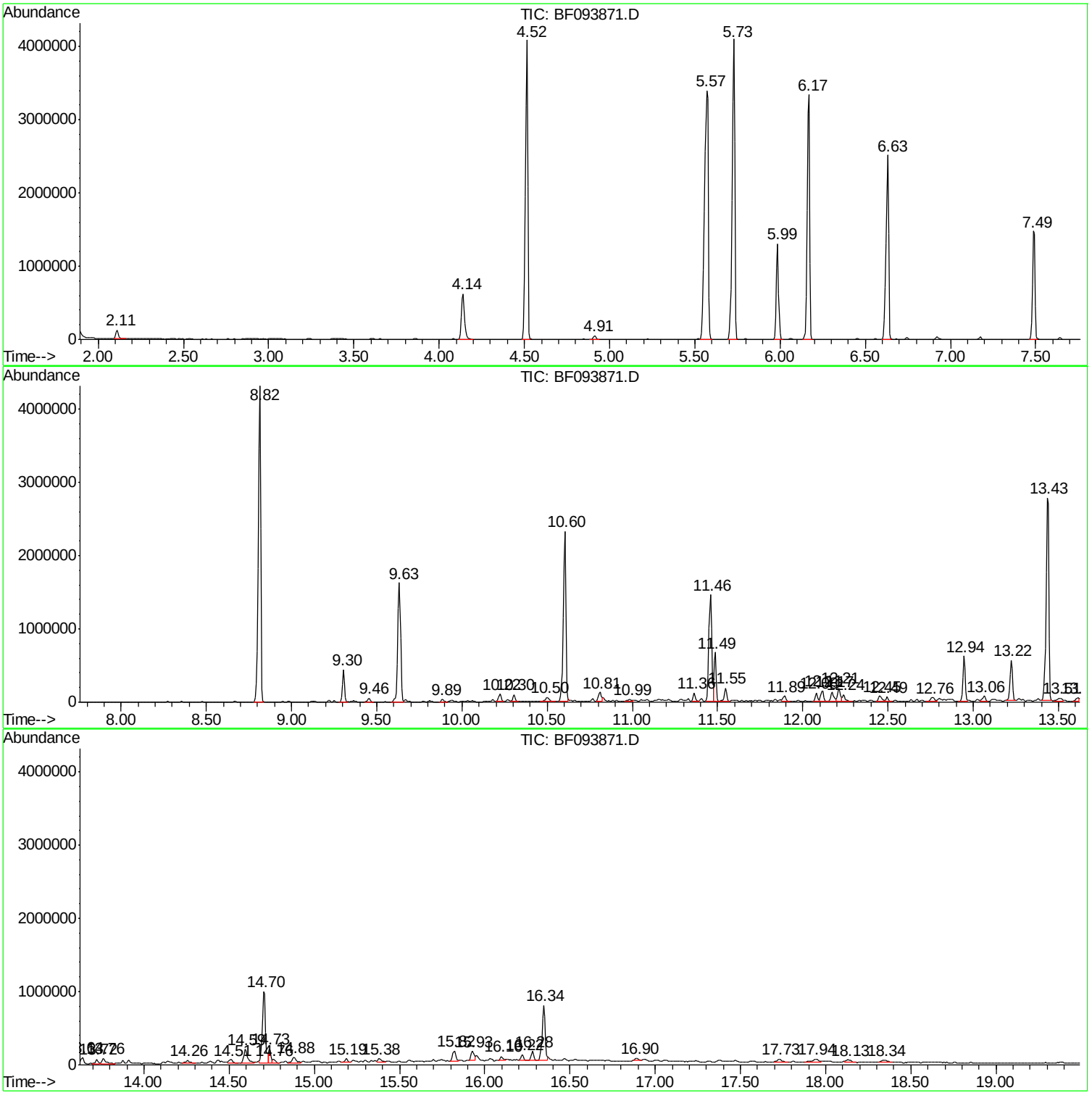
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093871.D
Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BF093871.D
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Sample : I2350-16
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Instrument :
BNA_F
ClientSampleId :
72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

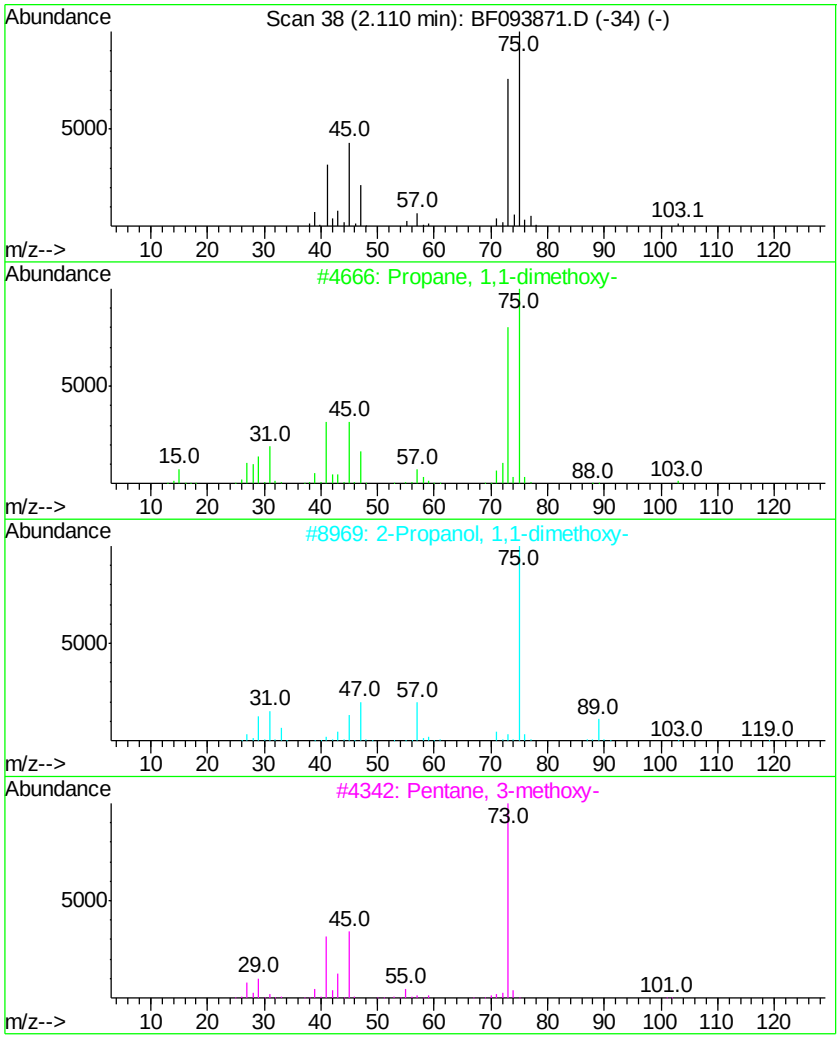
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

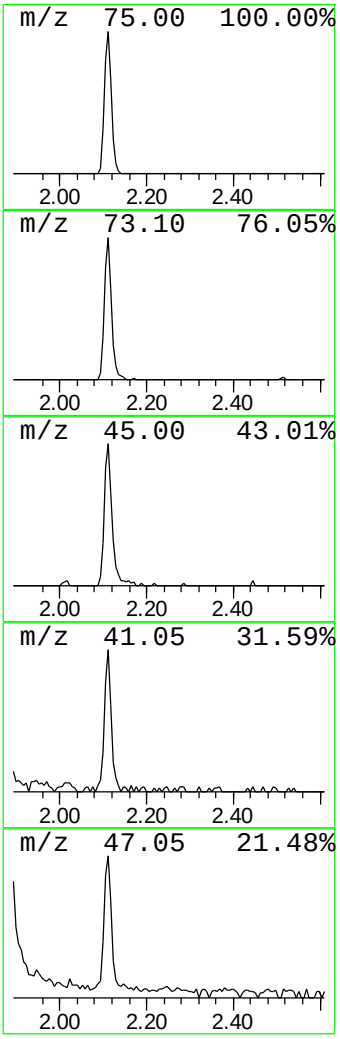
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	2.41 ng	140643	1,4-Dichlorobenzene-d4	5.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	28
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093871.D
Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

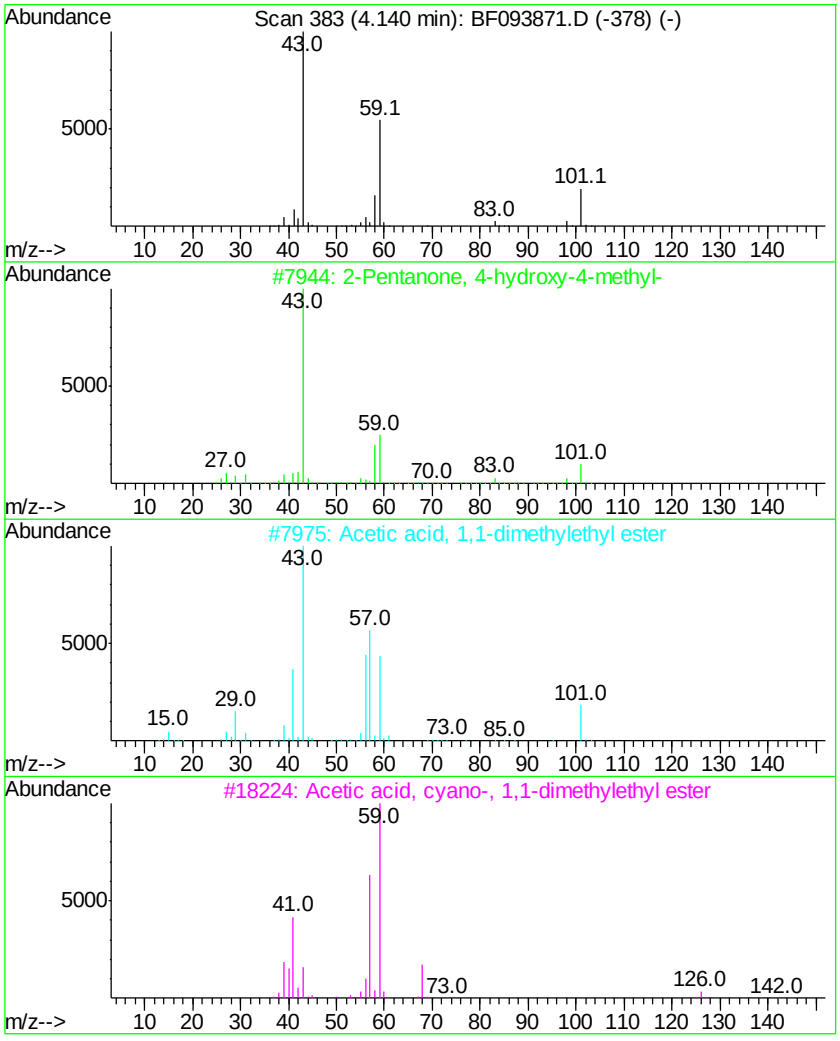
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

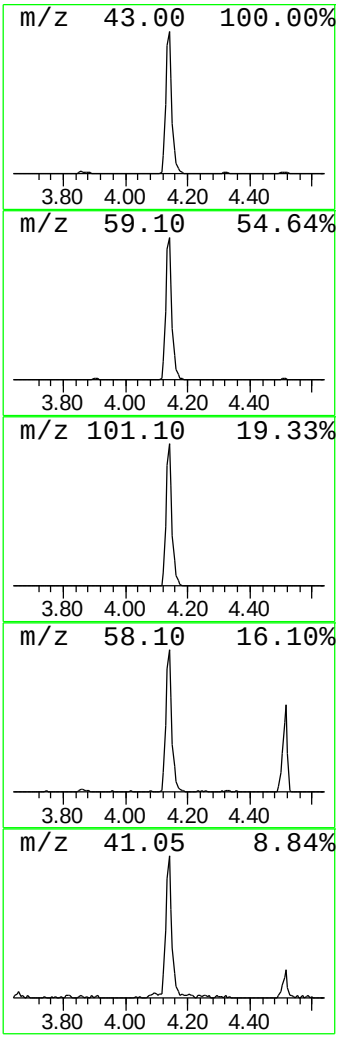
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	14.35 ng	837033	1,4-Dichlorobenzene-d4	5.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
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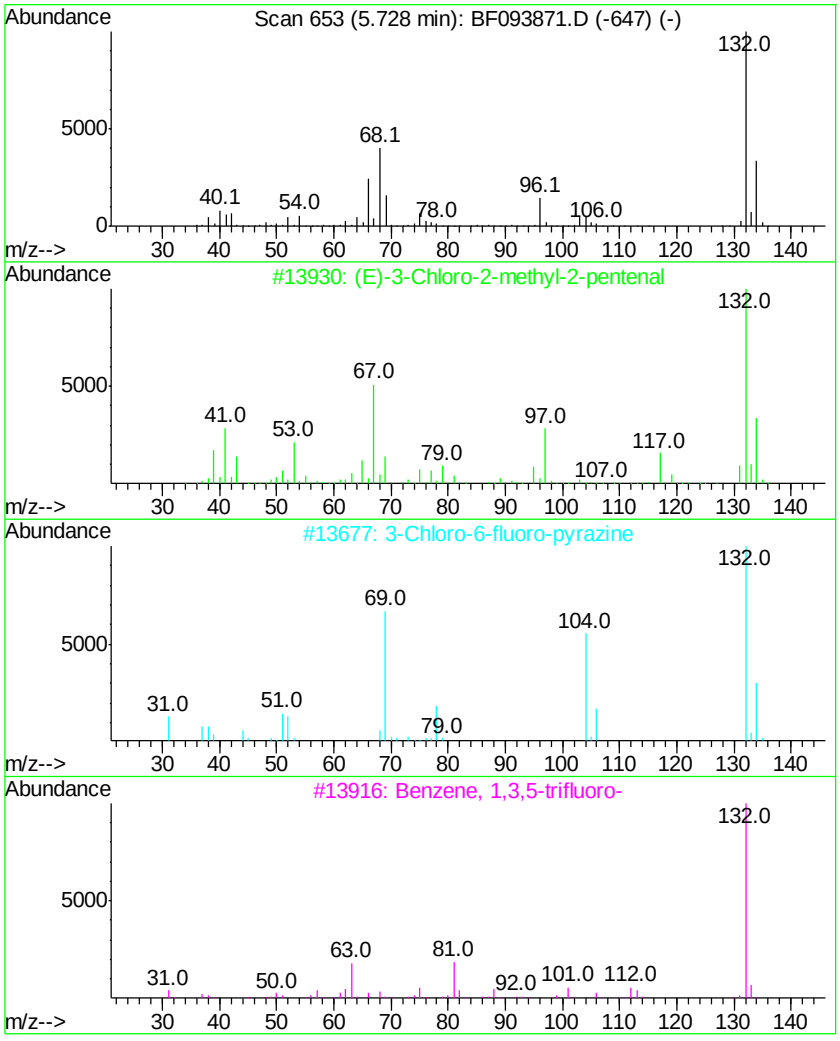
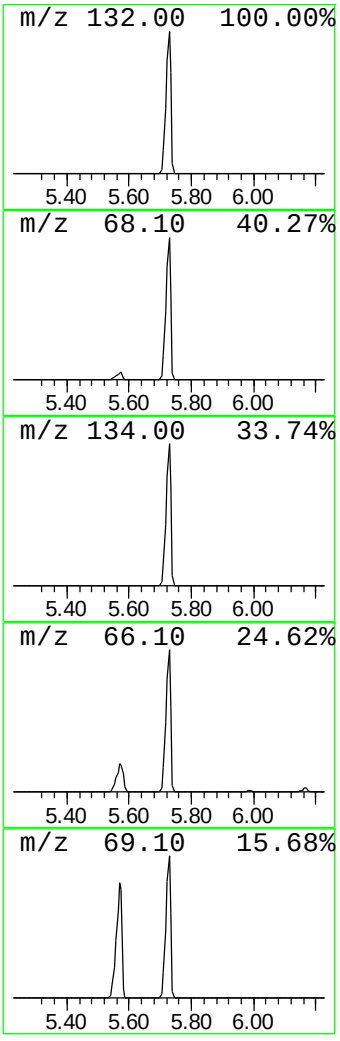
Peak Number 3 unknown5.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	78.64 ng	4586330	1,4-Dichlorobenzene-d4	5.99

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	16
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





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Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
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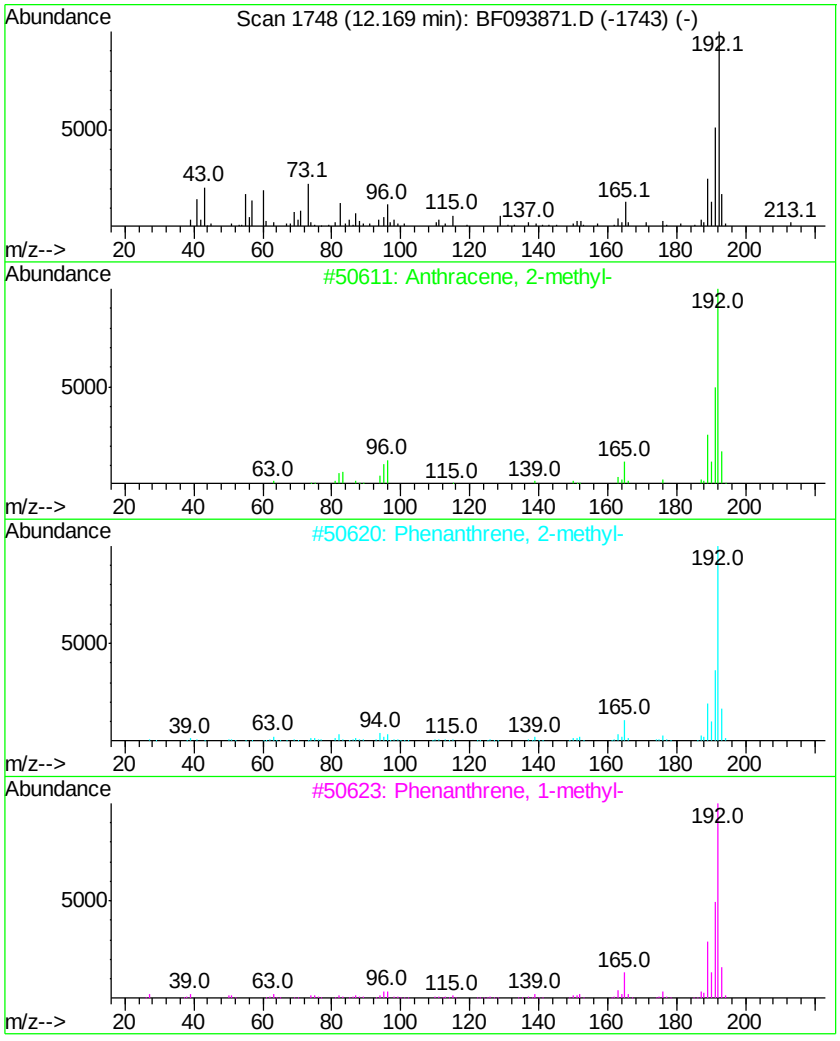
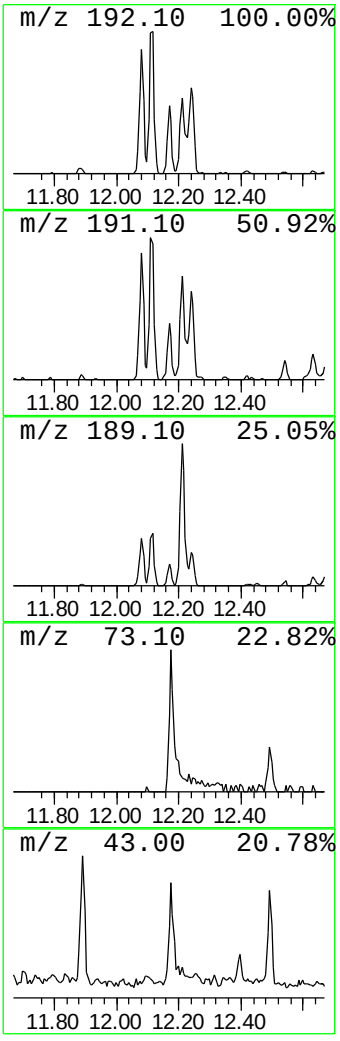
Peak Number 5 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	2.05 ng	155653	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	78





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Operator : SJ/MA
Sample : I2350-16
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Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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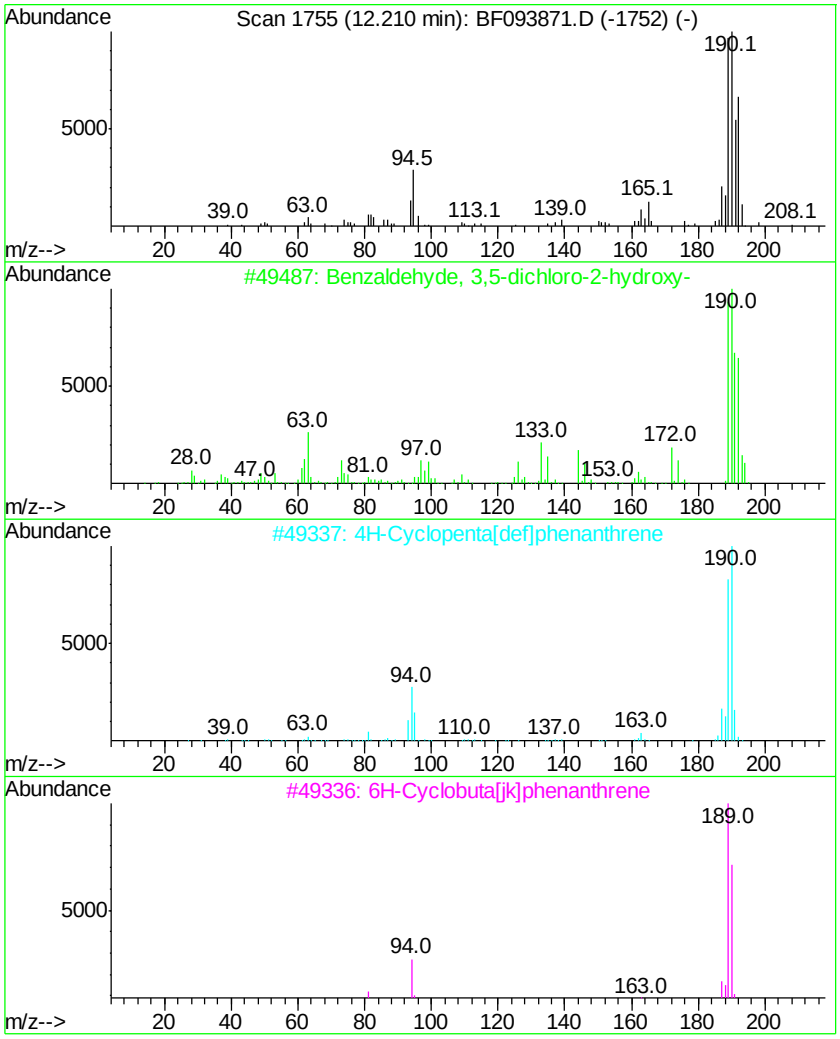
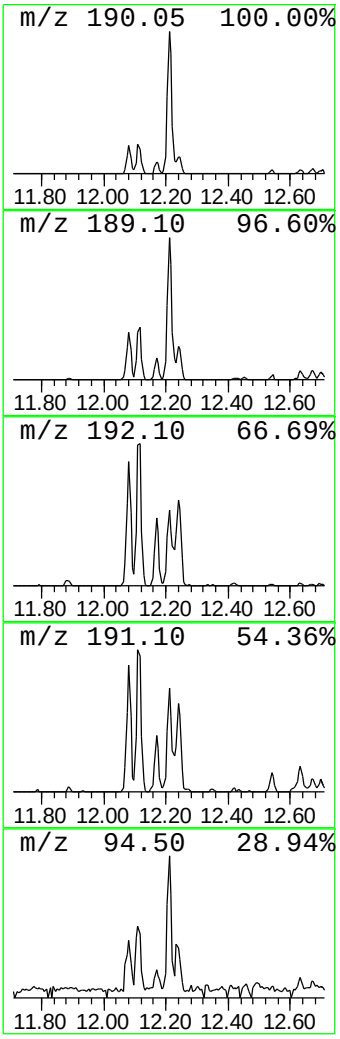
Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.21	2.75 ng	208194	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
5	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	30





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Misc :
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Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

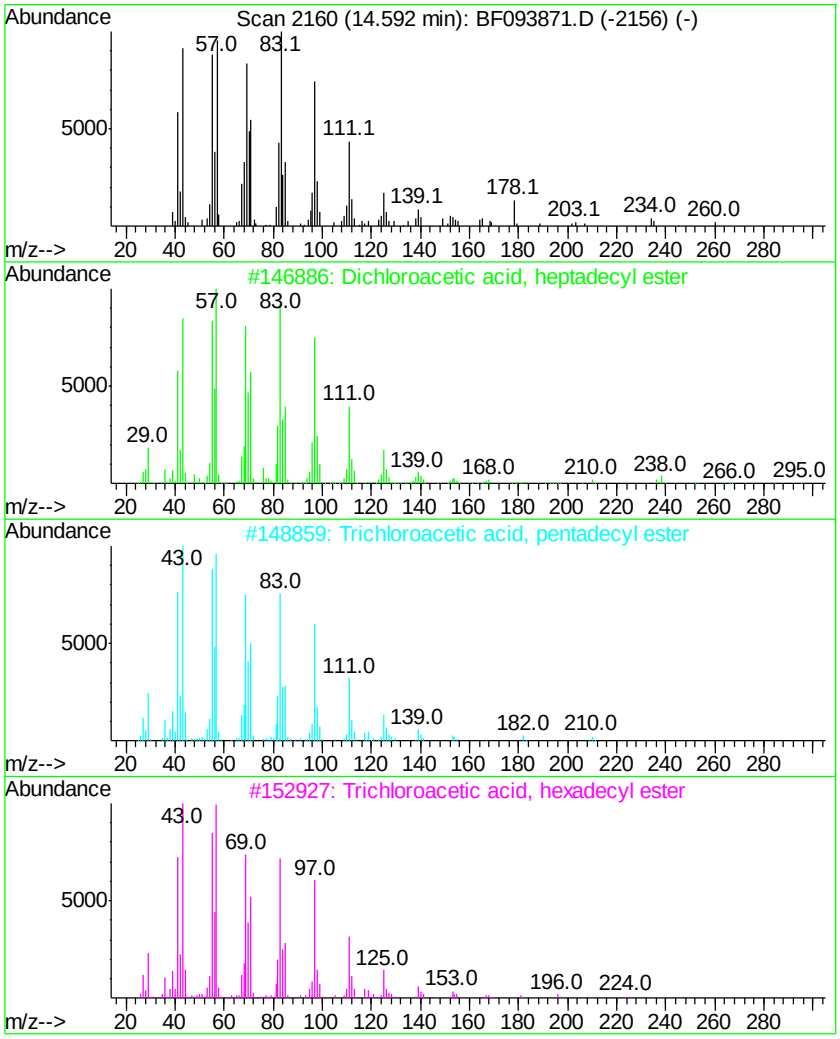
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

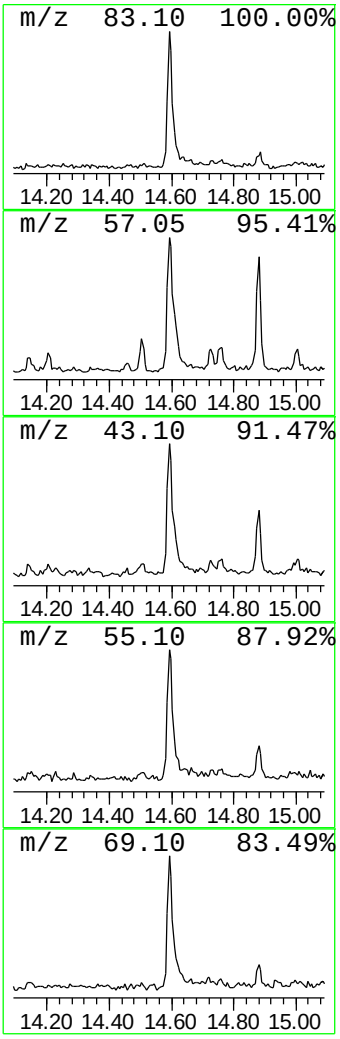
****

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	4.37 ng	287451	Chrysene-d12	14.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
5	1-Octadecanol	270	C18H38O	000112-92-5	90





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Data File : BF093871.D
Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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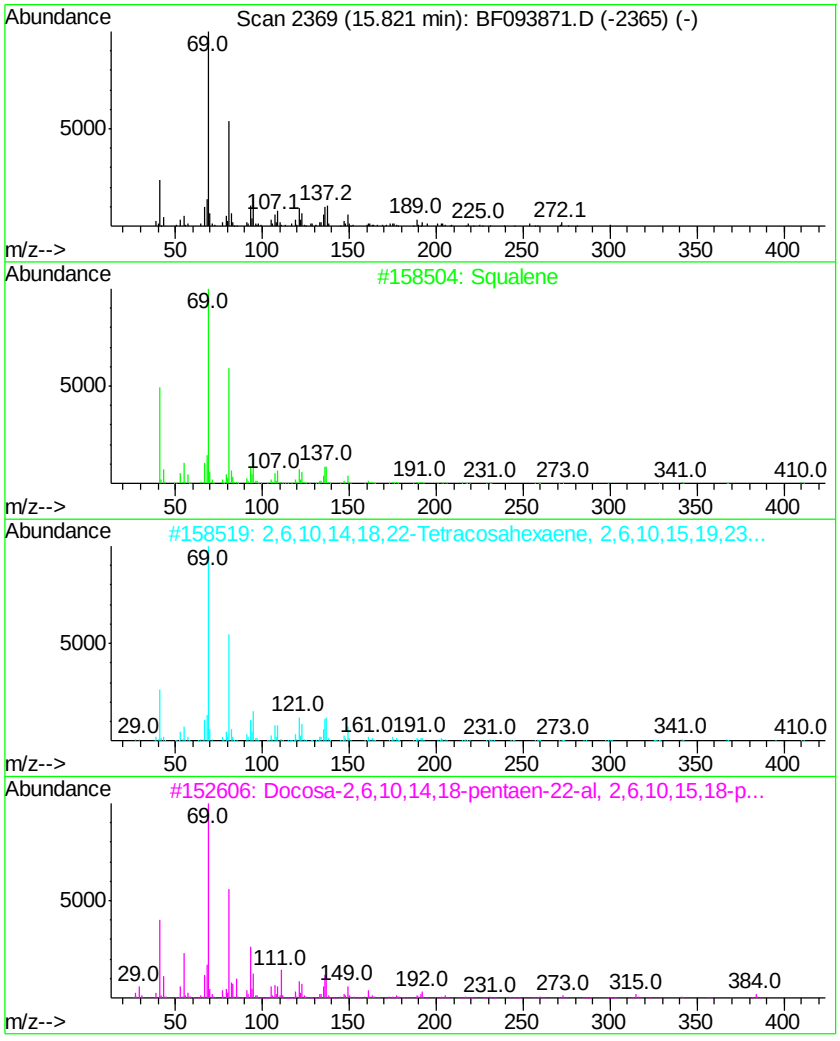
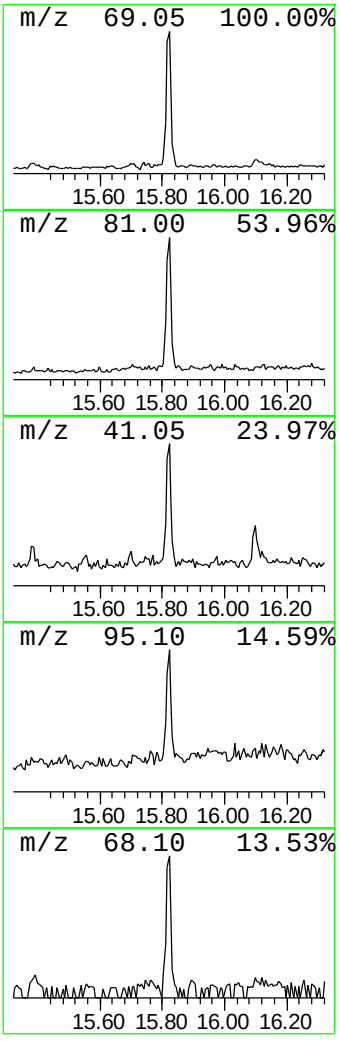
Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	3.36 ng	156548	Perylene-d12	16.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	87
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
5	(E,E,E)-3,7,11,15-Tetramethylhex...	272	C20H32	077898-97-6	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093871.D
Acq On : 23 Mar 2017 9:30
Operator : SJ/MA
Sample : I2350-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931-VNJ-226-213-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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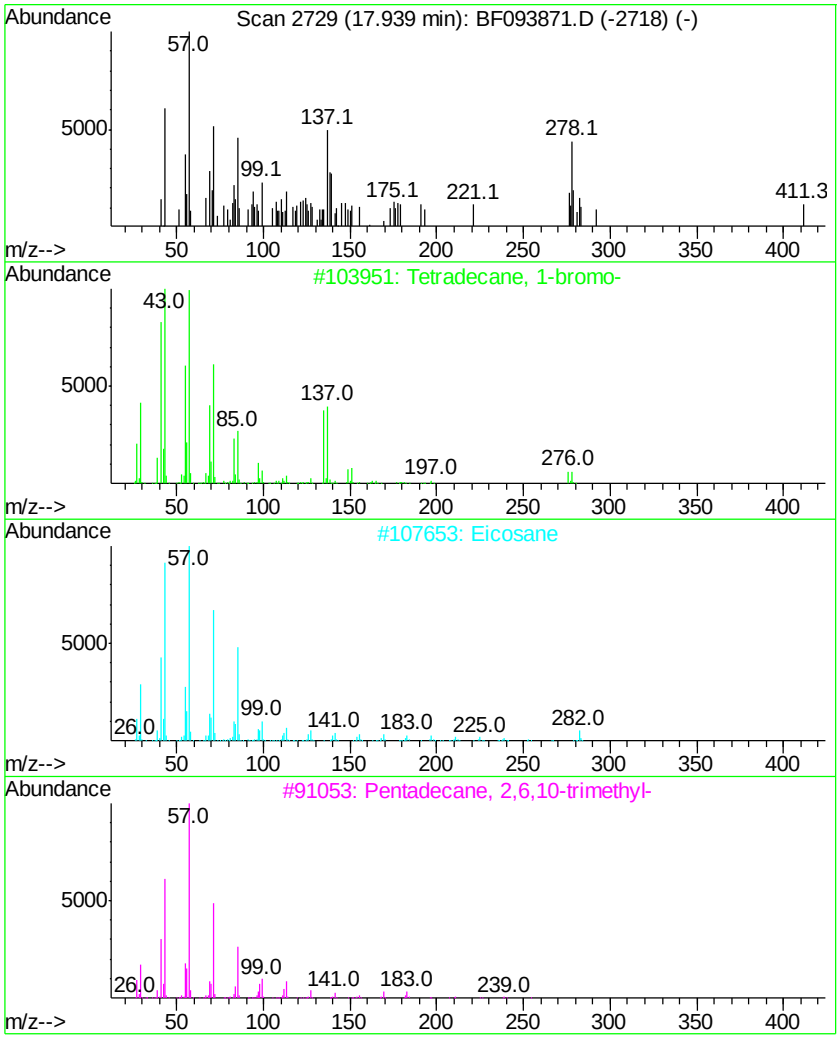
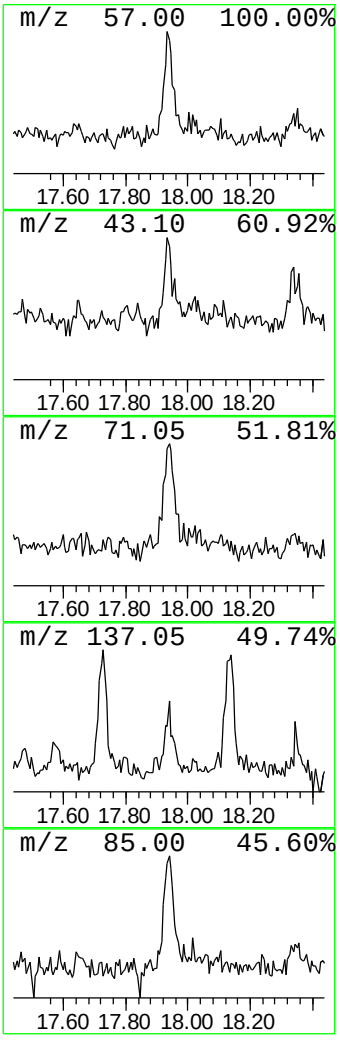
Peak Number 9 unknown17.94 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	2.64 ng	122942	Perylene-d12	16.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	38
2	Eicosane	282	C20H42	000112-95-8	25
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	11
4	(+)-Phendimetrazine	191	C12H17NO	000634-03-7	11
5	Undecane	156	C11H24	001120-21-4	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	2.11	2.4	ng	140643	1	5.99	1166480	20.0
2-Pentanone, 4-hy...	4.14	14.4	ng	837033	1	5.99	1166480	20.0
unknown5.73	5.73	78.6	ng	4586330	1	5.99	1166480	20.0
Anthracene, 2-met...	12.17	2.0	ng	155653	4	11.46	1515940	20.0
Benzaldehyde, 3,5...	12.21	2.8	ng	208194	4	11.46	1515940	20.0
Dichloroacetic ac...	14.59	4.4	ng	287451	5	14.71	1315290	20.0
Squalene	15.82	3.4	ng	156548	6	16.34	932847	20.0
unknown17.94	17.94	2.6	ng	122942	6	16.34	932847	20.0