LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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	4.645	465	469	478	rBV	192618	302838	10.83%	1.351%
2	4.716	478	481	491	rVB	38293	45378	1.62%	0.202%
3	5.098	542	546	559	rBV	2416595	2501641	89.47%	11.163%
4	6.163	720	727	737	rBV	2477724	2796207	100.00%	12.477%
5	6.239	737	740	741	rBV	52853	46227	1.65%	0.206%
6	6.269	741	745	748	rVB	2621049	2390755	85.50%	10.668%
7	6.492	780	783	791	rBV	730214	639516	22.87%	2.854%
8	6.651	806	810	813	rBV	1837810	1647530	58.92%	7.352%
9	6.828	836	840	846	rVB	40324	43617	1.56%	0.195%
10	7.063	872	880	883	rBV	1636381	1593927	57.00%	7.113%
11	7.275	912	916	919	rBV	27754	28736	1.03%	0.128%
12	7.775	997	1001	1005	rBV	1001594	945428	33.81%	4.219%
13	8.492	1118	1123	1126	rVB	46410	45800	1.64%	0.204%
14	8.586	1136	1139	1142	rBV	55090	44763	1.60%	0.200%
15	8.857	1180	1185	1188	rBV	2327842	2049197	73.28%	9.144%
16	9.122	1225	1230	1234	rBV	33425	52443	1.88%	0.234%
17	9.192	1238	1242	1244	rVV2	41031	52224	1.87%	0.233%
18	9.257	1248	1253	1255	rVV	347092	302204	10.81%	1.349%
19	9.304	1258	1261	1266	rVB6	23176	35288	1.26%	0.157%
20	9.386	1272	1275	1279	rBV6	23955	40881	1.46%	0.182%
21	9.522	1294	1298	1302	rBV	972801	954767	34.15%	4.260%
22	9.633	1314	1317	1322	rBV5	24440	37475	1.34%	0.167%
23	9.733	1332	1334	1337	rBV2	29757	32211	1.15%	0.144%
24	9.845	1350	1353	1356	rBV4	25898	32673	1.17%	0.146%
25	9.980	1373	1376	1378	rBV	72190	54735	1.96%	0.244%
26	10.198	1409	1413	1416	rBV2	33006	41824	1.50%	0.187%
27	10.310	1428	1432	1439	rBV	1213108	1108123	39.63%	4.945%
28	10.433	1450	1453	1454	rBV2	34531	37343	1.34%	0.167%
29	10.451	1454	1456	1457	rBV	52959	41980	1.50%	0.187%
30	10.898	1530	1532	1534	rVB	44071	30681	1.10%	0.137%
31	10.998	1545	1549	1558	rVB	950913	822868	29.43%	3.672%
32	11.074	1558	1562	1565	rBV3	26518	37271	1.33%	0.166%
33	11.321	1601	1604	1610	rBV2	26550	39573	1.42%	0.177%
34	11.498	1626	1634	1638	rBV7	40210	122434	4.38%	0.546%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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	11.557	1641	1644	1647	rBV	114120	97642	3.49%	0.436%
36	11.639	1656	1658	1663	rVB5	30866	31696	1.13%	0.141%
37	11.745	1672	1676	1680	rVB3	164462	171101	6.12%	0.763%
38	11.857	1691	1695	1697	rBV	106562	94490	3.38%	0.422%
39	12.257	1758	1763	1775	rVV4	95465	243338	8.70%	1.086%
40	12.339	1775	1777	1782	rVV4	46501	51154	1.83%	0.228%
41	12.586	1815	1819	1822	rBV	1229773	1173801	41.98%	5.238%
42	12.721	1838	1842	1844	rBV2	28992	29495	1.05%	0.132%
43	12.963	1881	1883	1891	rBV4	46649	53133	1.90%	0.237%
44	13.498	1971	1974	1981	rVB2	110049	130037	4.65%	0.580%
45	13.621	1992	1995	1999	rBV	520708	499434	17.86%	2.229%
46	13.933	2046	2048	2053	rBV6	38793	78474	2.81%	0.350%
47	14.939	2217	2219	2221	rBV3	29870	30184	1.08%	0.135%
48	14.974	2221	2225	2231	rVB	473465	551582	19.73%	2.461%
49	15.562	2322	2325	2328	rBV4	38456	59072	2.11%	0.264%
50	16.174	2426	2429	2430	rBV3	27562	37426	1.34%	0.167%
51	17.509	2654	2656	2664	rVB8	24315	36918	1.32%	0.165%
52	17.727	2691	2693	2701	rVB8	26686	42589	1.52%	0.190%

Sum of corrected areas: 22410124

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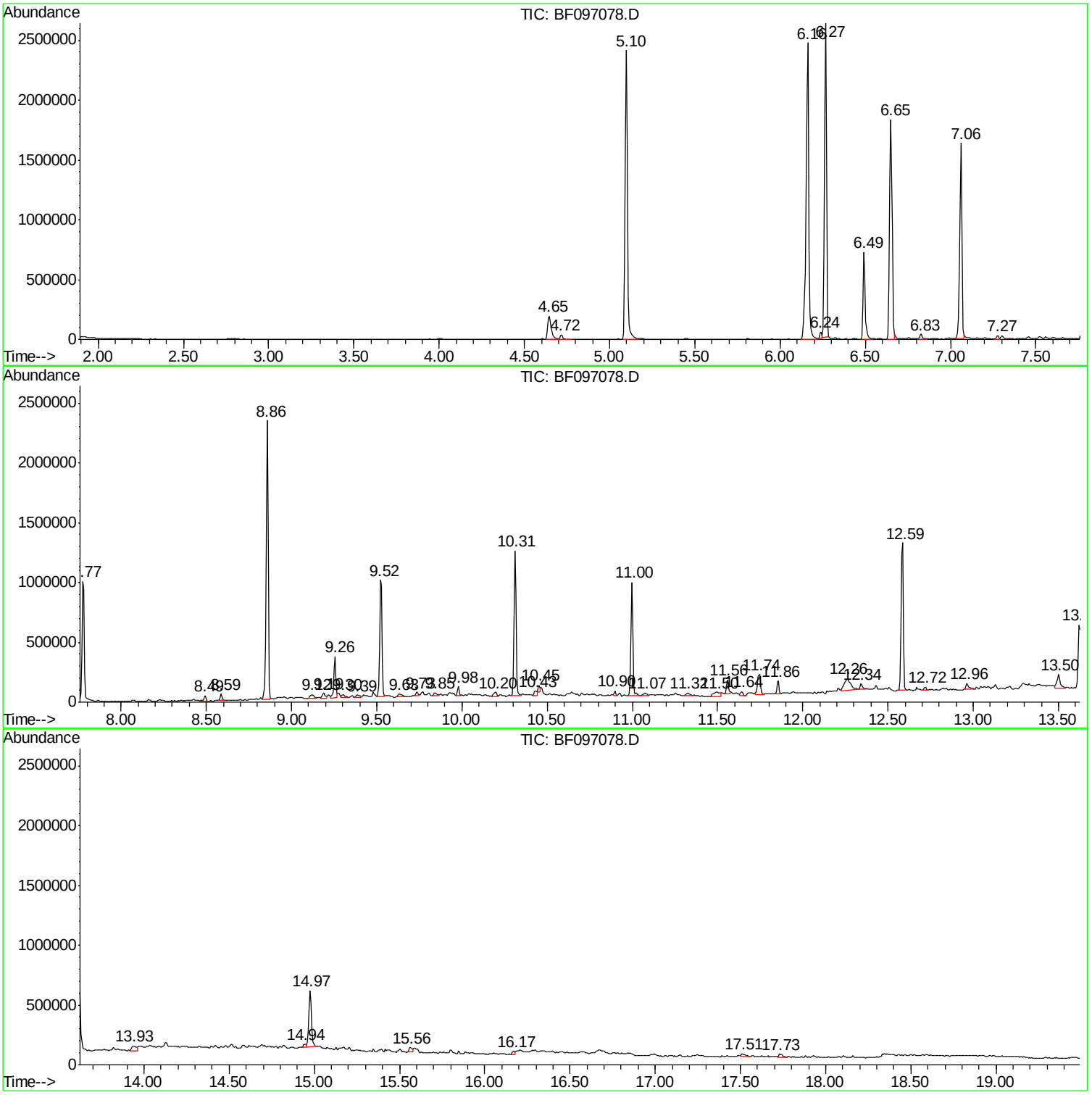
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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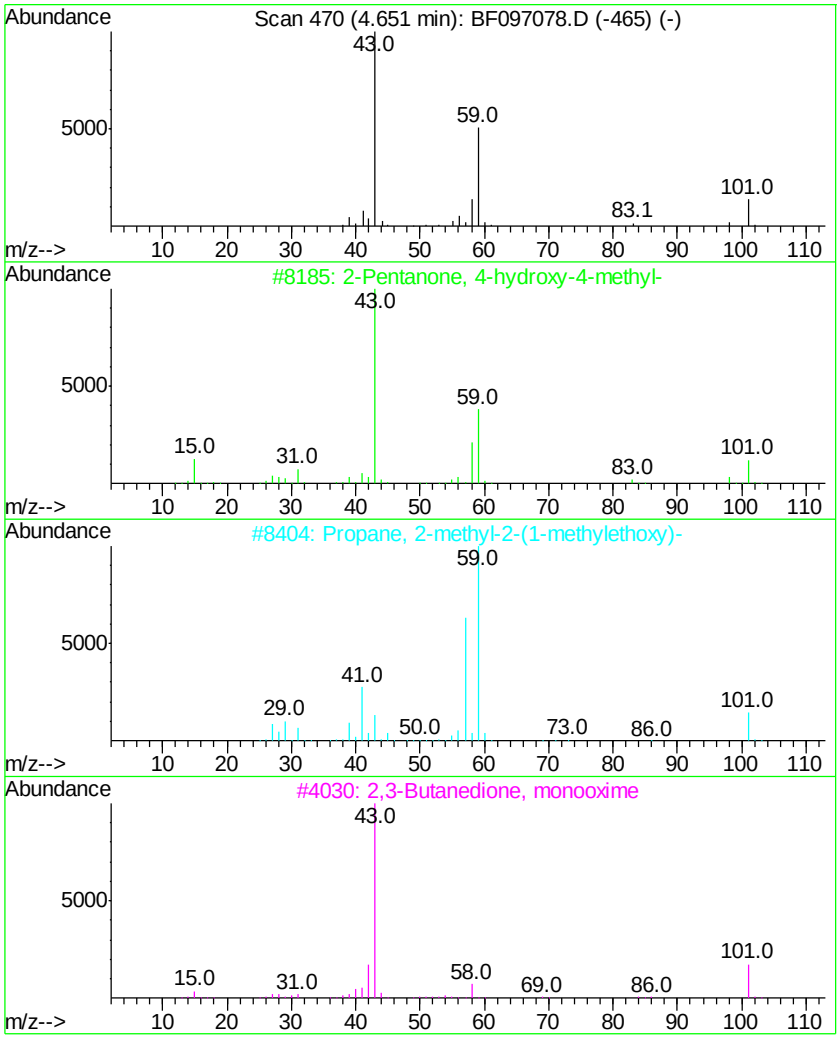
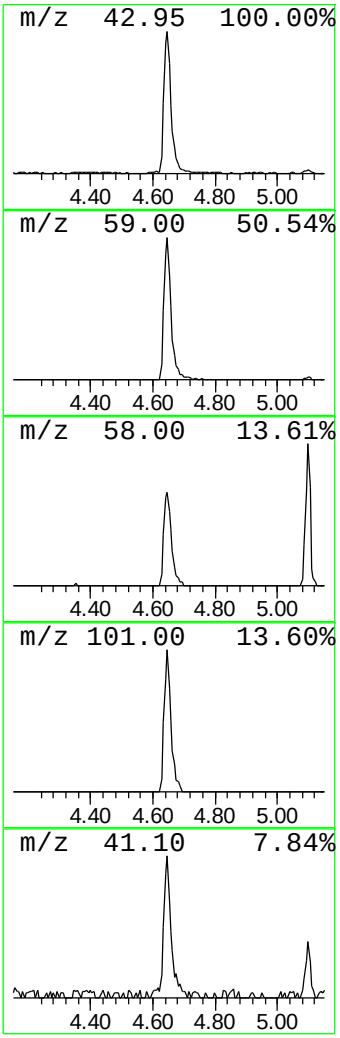
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	9.47 ng	302838	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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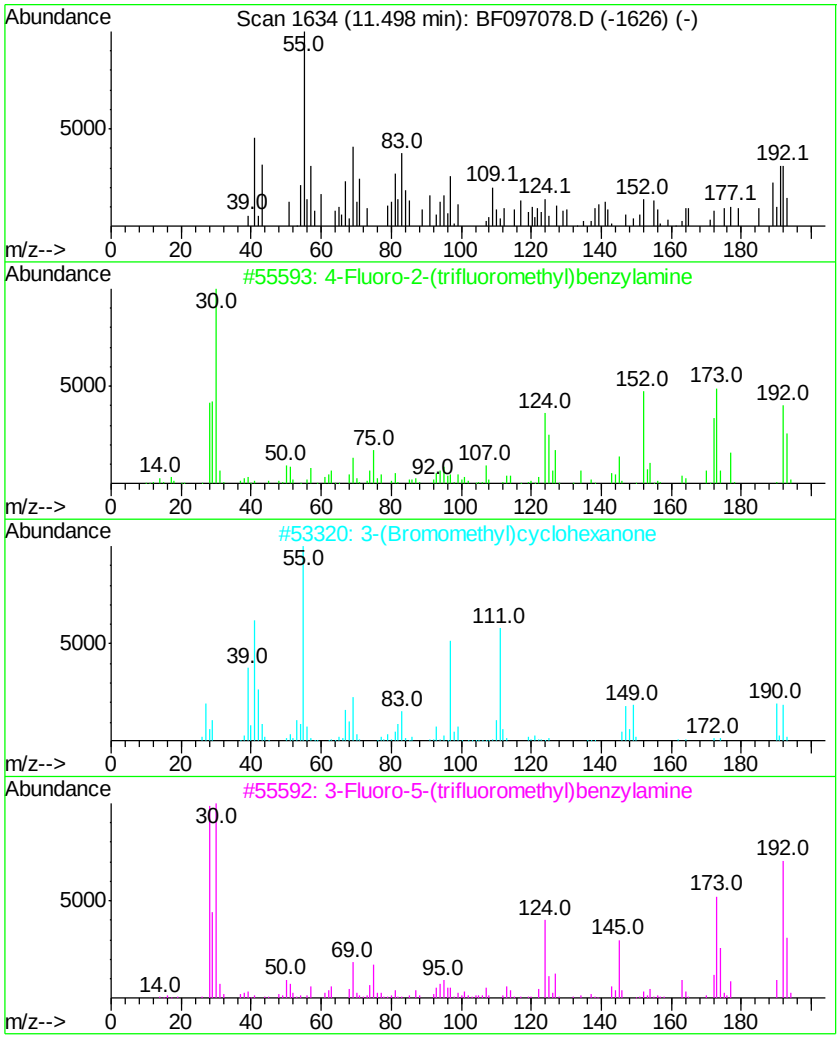
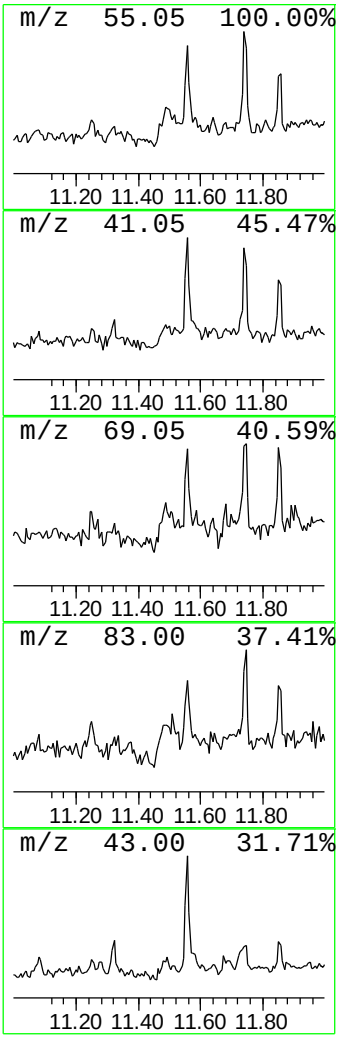
Peak Number 3 unknown11.50 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	2.98 ng	122434	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-2-(trifluoromethyl)benz...	193	C8H7F4N	202522-22-3	9
2	3-(Bromomethyl)cyclohexanone	190	C7H11BrO	168278-83-9	9
3	3-Fluoro-5-(trifluoromethyl)benz...	193	C8H7F4N	150517-77-4	9
4	4-Fluoro-3-(trifluoromethyl)benz...	193	C8H7F4N	067515-74-6	9
5	Bicyclo(3.3.1)nonane-2,6-dione	152	C9H12O2	016473-11-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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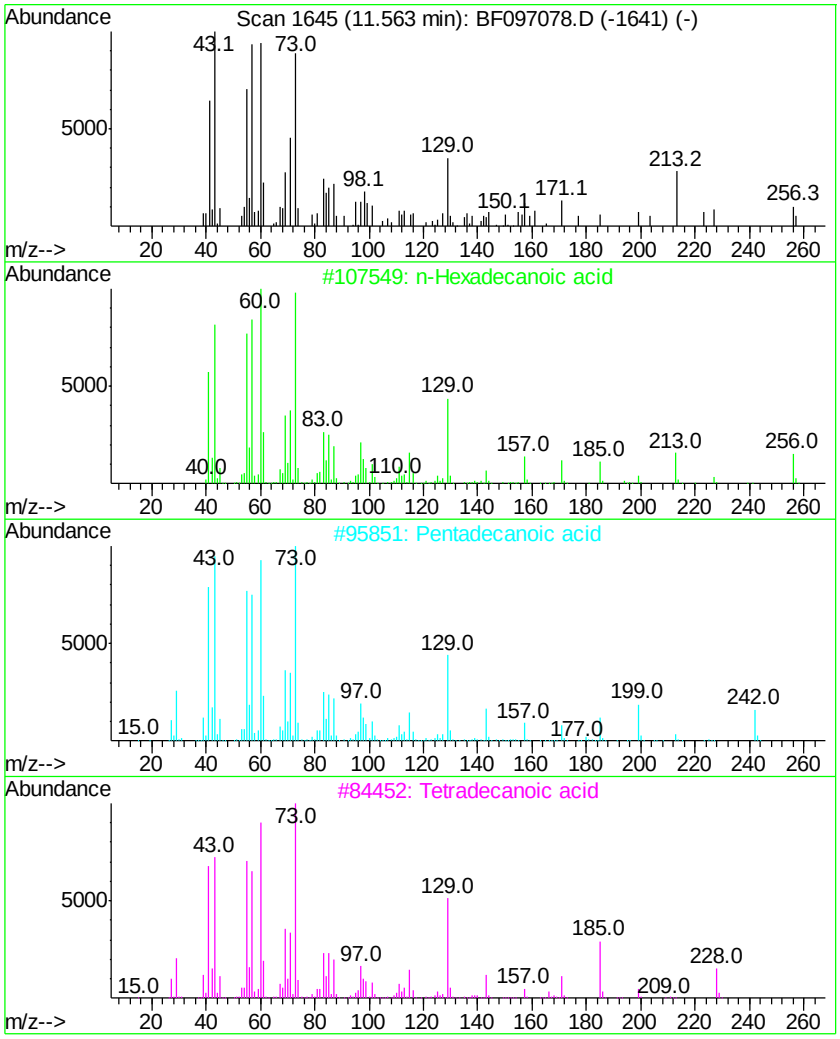
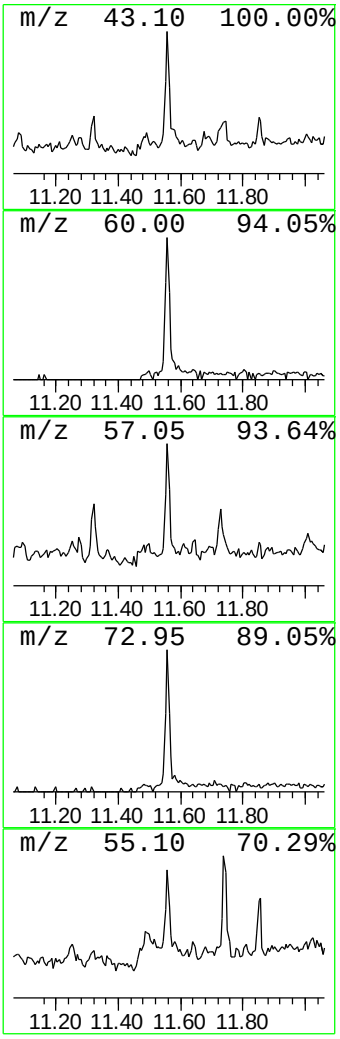
Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	2.37 ng	97642	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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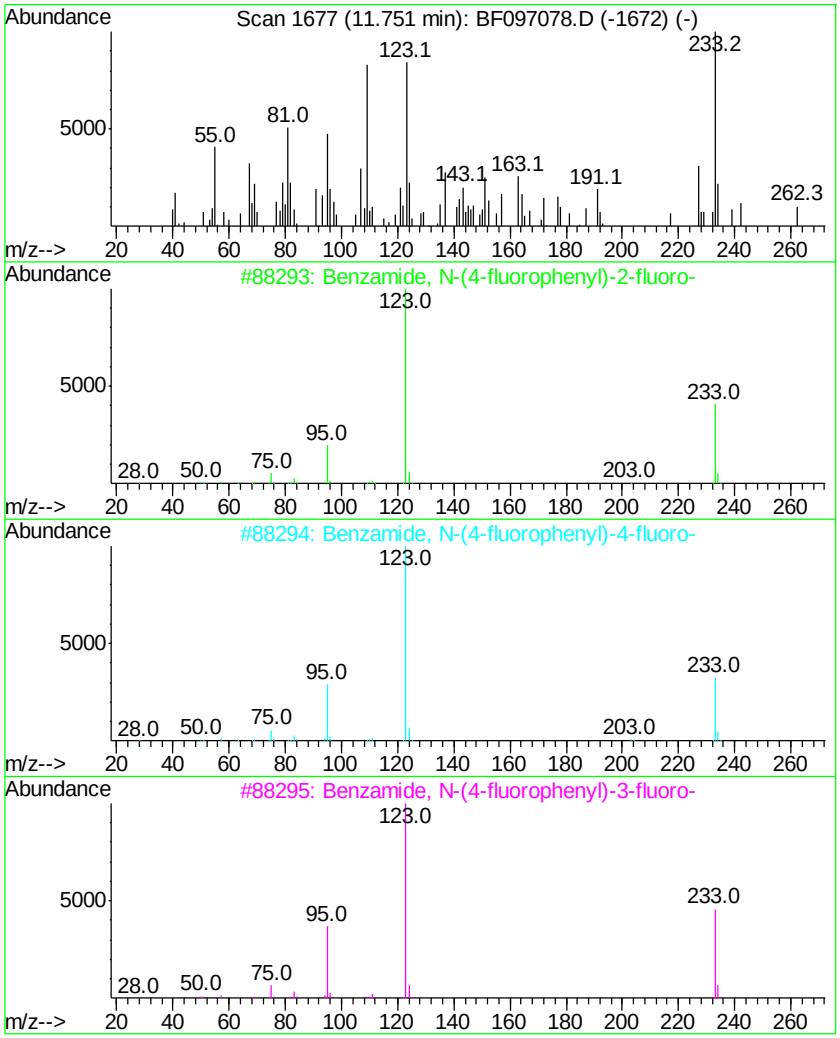
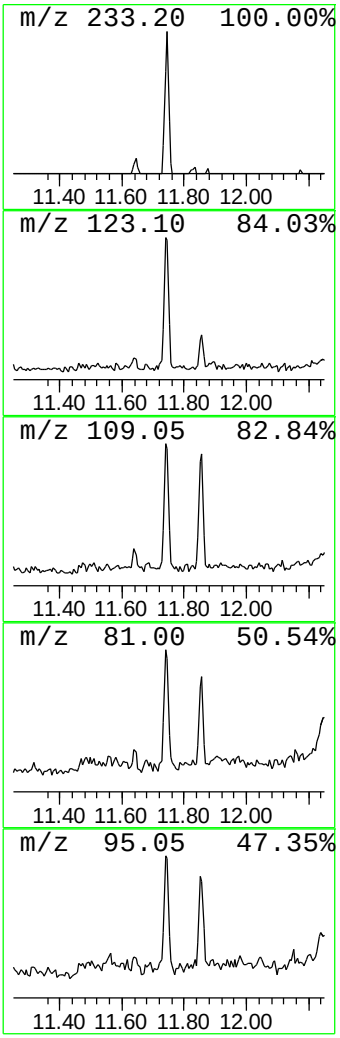
Peak Number 5 unknown11.75 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.16 ng	171101	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-(4-fluorophenyl)-2-...	233	C13H9F2NO	1000307-07-9	43
2	Benzamide, N-(4-fluorophenyl)-4-...	233	C13H9F2NO	1000307-10-1	43
3	Benzamide, N-(4-fluorophenyl)-3-...	233	C13H9F2NO	1000307-16-3	43
4	2-(3,3-Dimethyl-oxiran-2-yl)-5-e...	209	C11H15NO3	1000194-95-4	25
5	3-Pyridinol, 2,6-dimethyl-	123	C7H9NO	001122-43-6	11





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Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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

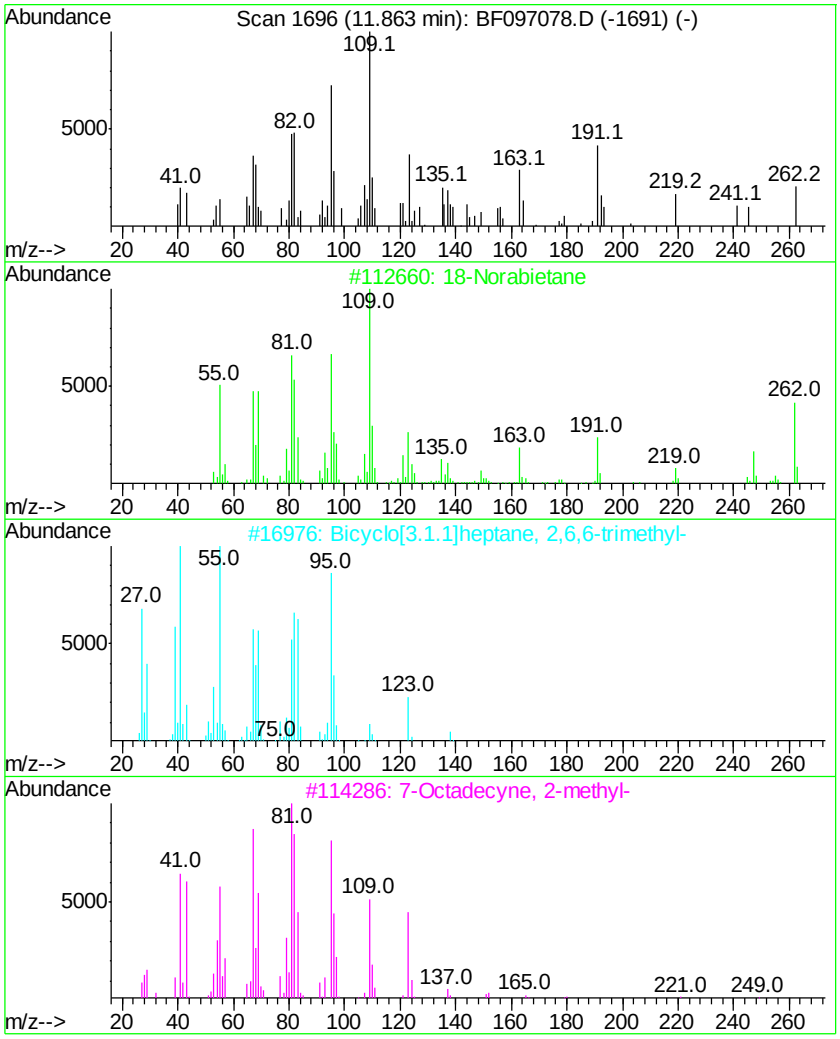
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

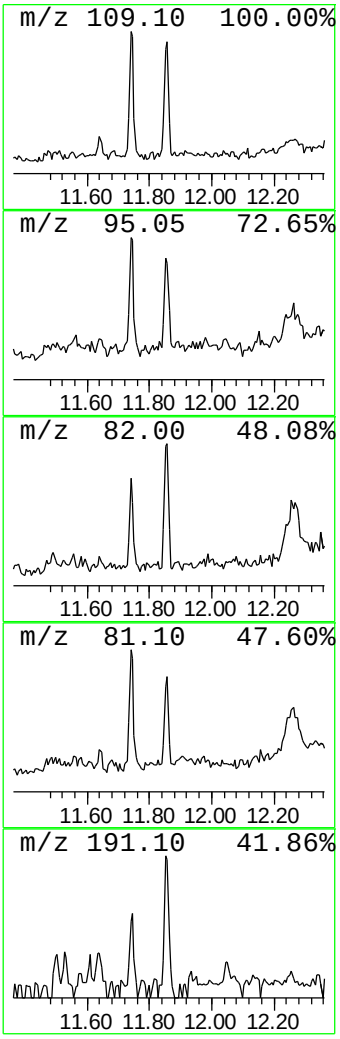
****

Peak Number 6 18-Norabietane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.30 ng	94490	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Norabietane	262	C19H34	1000293-16-6	94
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	38
3	7-Octadecyne, 2-methyl-	264	C19H36	035354-38-2	38
4	1H-Pyrazol-5-amine, 1-[(4-fluoro...	191	C10H10FN3	1000362-66-0	30
5	1a,2,5,5-Tetramethyl-cis-1a,4a,5...	194	C13H22O	1000215-77-7	27





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Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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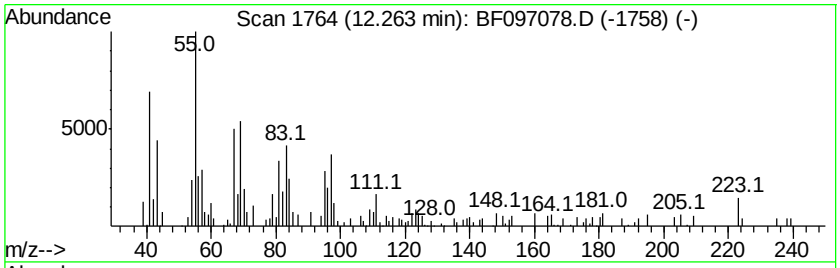
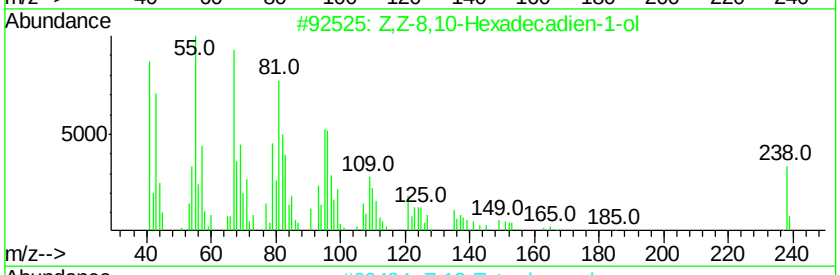
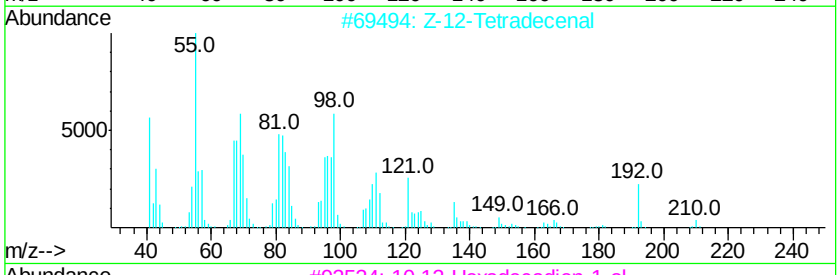
Peak Number 7 unknown12.26 Concentration Rank 3

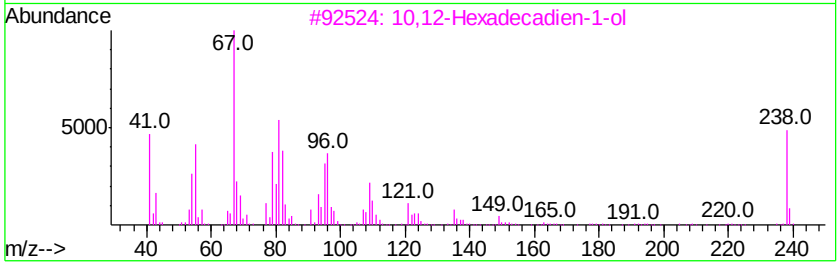
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	5.91 ng	243338	Phenanthrene-d10	11.00

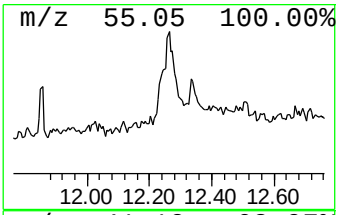
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z,Z-8,10-Hexadecadien-1-ol	238	C16H30O	1000130-91-0	38
2	Z-12-Tetradecenal	210	C14H26O	1000130-76-5	38
3	10,12-Hexadecadien-1-ol	238	C16H30O	1000130-89-7	38
4	1-Nonylcycloheptane	224	C16H32	1000371-47-7	25
5	1-Oxaspiro[2.5]octane-2-carbonit...	137	C8H11NO	036929-66-5	22

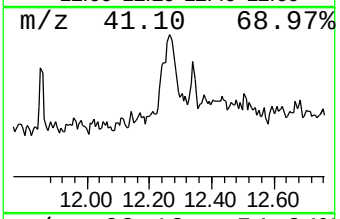


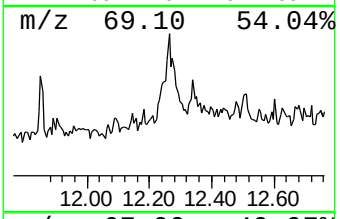


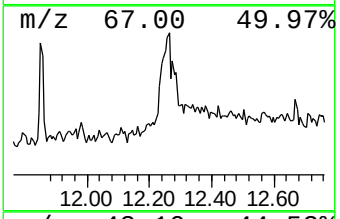


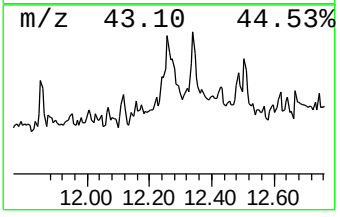












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Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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

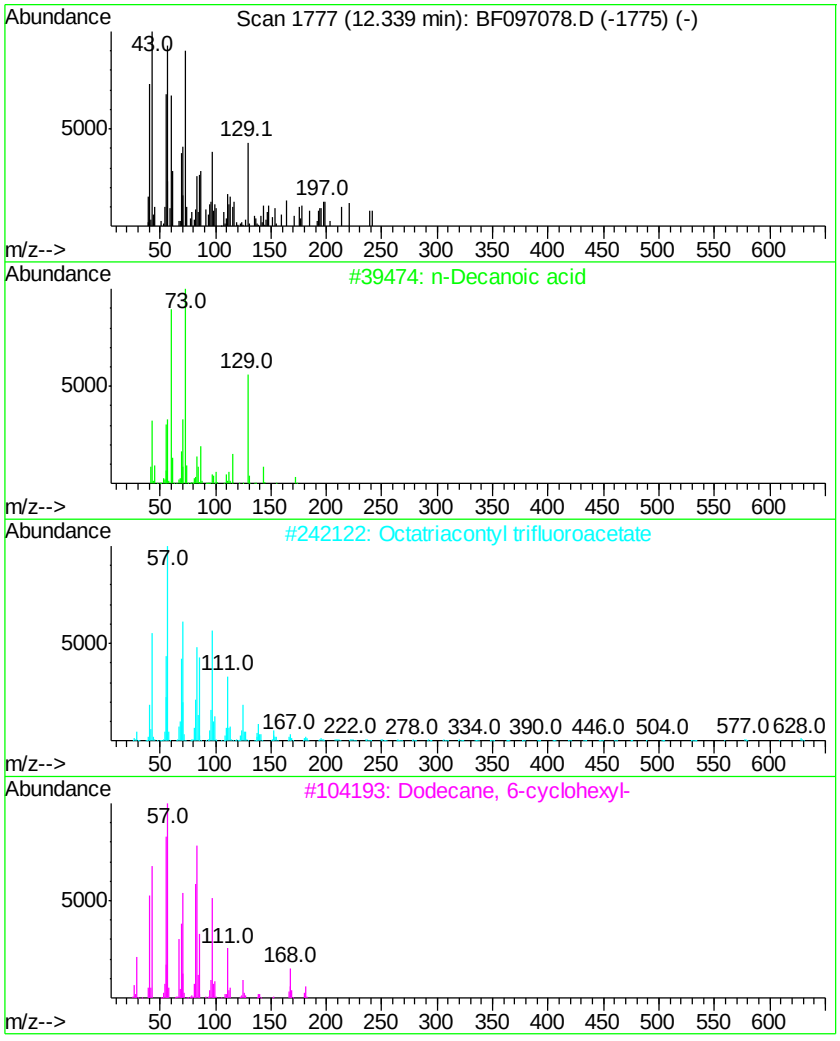
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

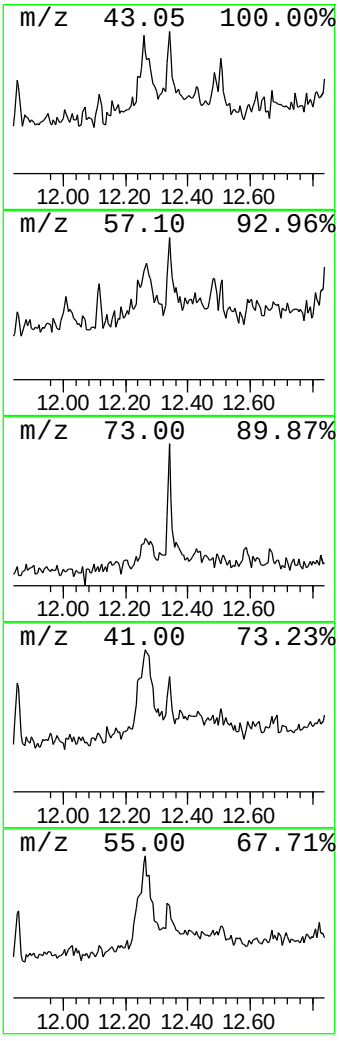
****

Peak Number 8 unknown12.34 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	2.05 ng	51154	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	43
2	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	22
3	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	22
4	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	14
5	Nonanoic acid	158	C9H18O2	000112-05-0	14





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Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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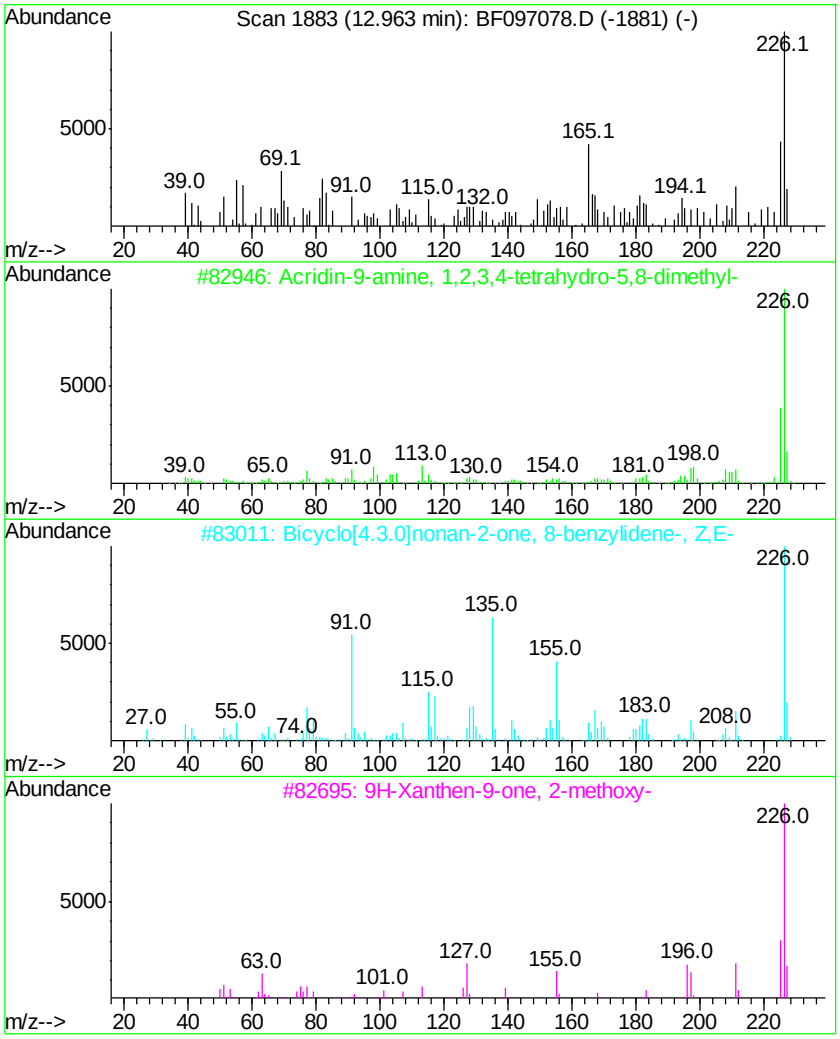
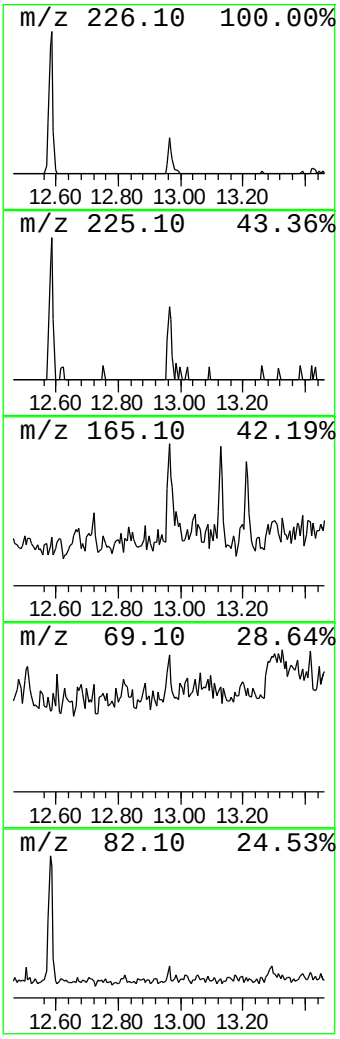
Peak Number 9 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	2.13 ng	53133	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	50
2	Bicyclo[4.3.0]nonan-2-one, 8-ben...	226	C16H18O	1000154-07-2	50
3	9H-Xanthen-9-one, 2-methoxy-	226	C14H10O3	001214-20-6	47
4	1-Ethyl-4-methoxy-9H-pyrido[3,4-...	226	C14H14N2O	026585-14-8	47
5	1,3-Diamino-5,6-dihydro-7-methyl...	226	C13H14N4	037436-37-6	46





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Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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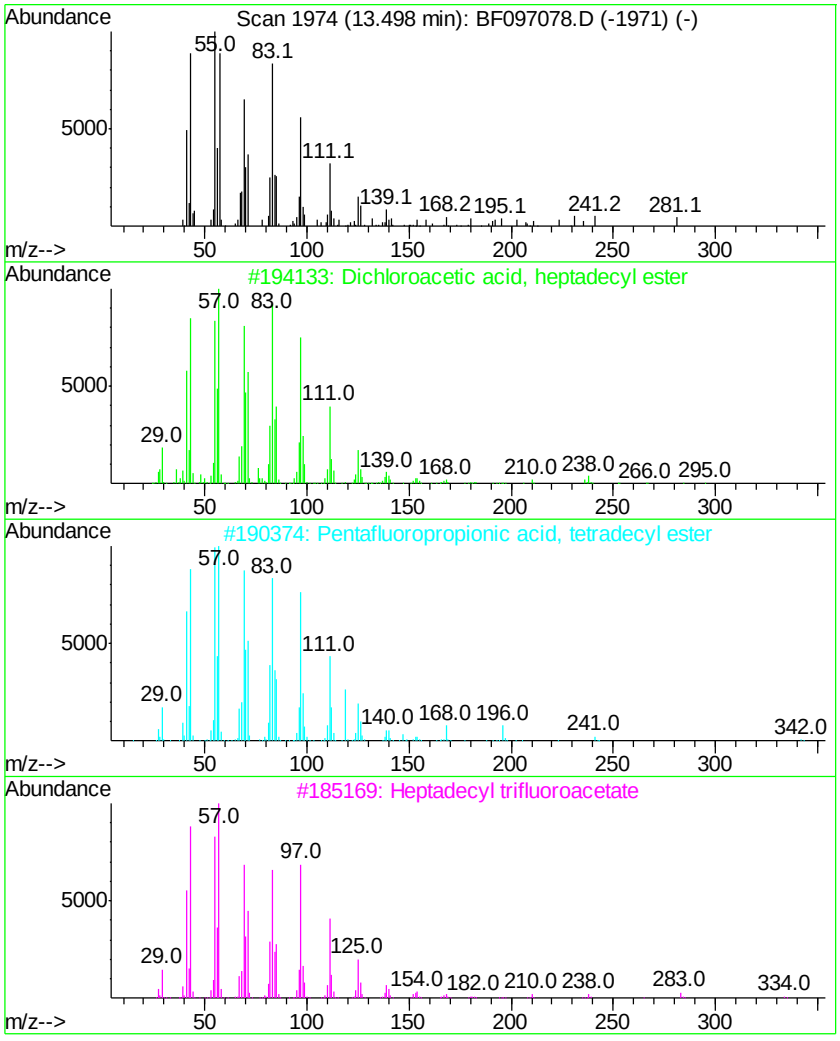
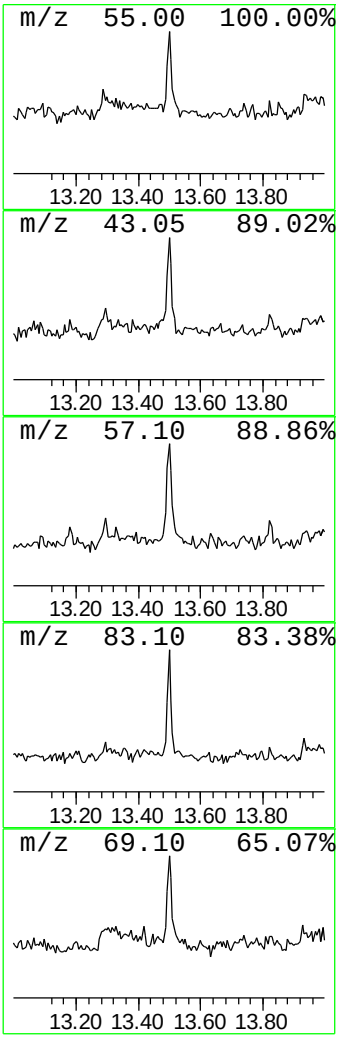
Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.21 ng	130037	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	68
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	68
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	68
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	68





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Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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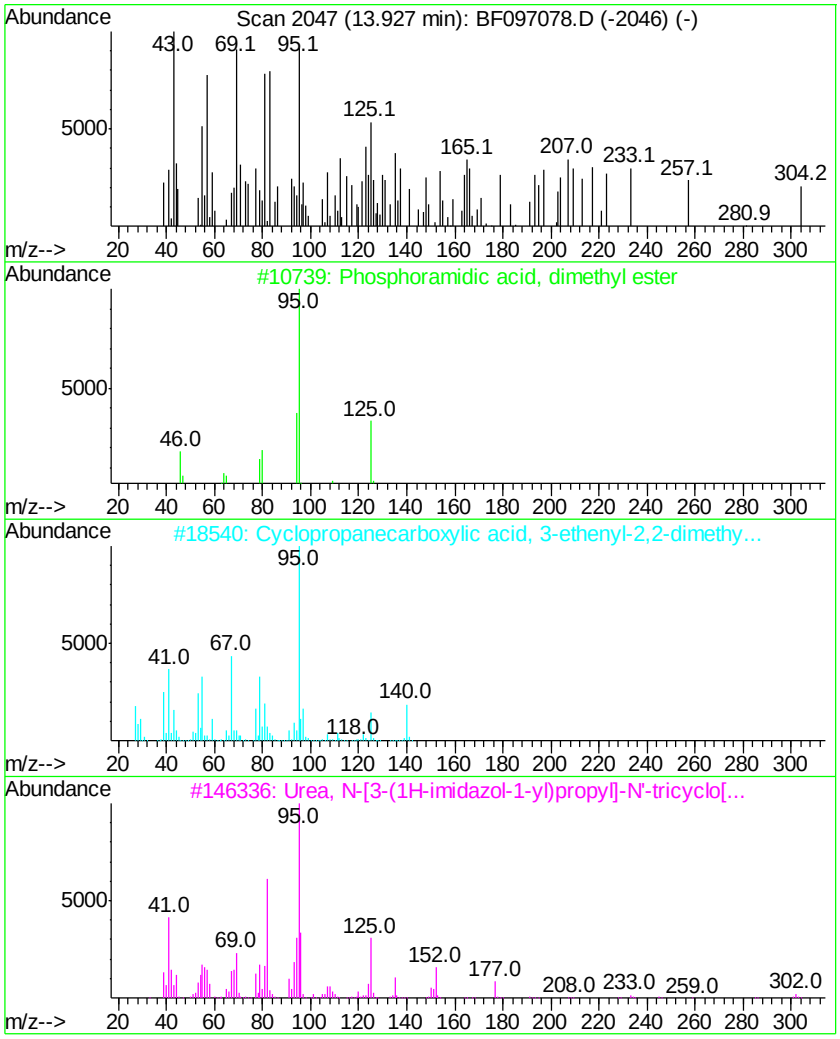
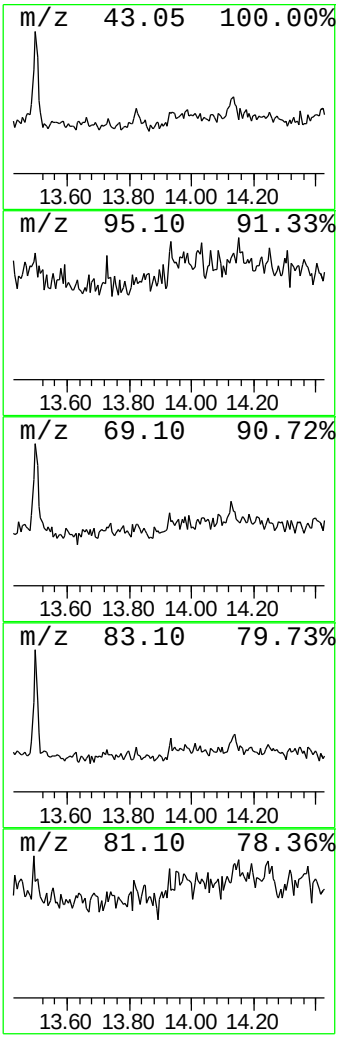
Peak Number 11 unknown13.93 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.14 ng	78474	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoramidic acid, dimethyl ester	125	C2H8NO3P	002697-42-9	22
2	Cyclopropanecarboxylic acid, 3-e...	140	C8H12O2	067528-58-9	14
3	Urea, N-[3-(1H-imidazol-1-yl)pro...	302	C17H26N4O	1000316-51-4	12
4	Cis-3-ethyl-endo-tricyclo[5.2.1....	164	C12H20	1000215-29-1	12
5	5-Octen-2-ol, 5-methyl-	142	C9H18O	118989-20-1	11





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Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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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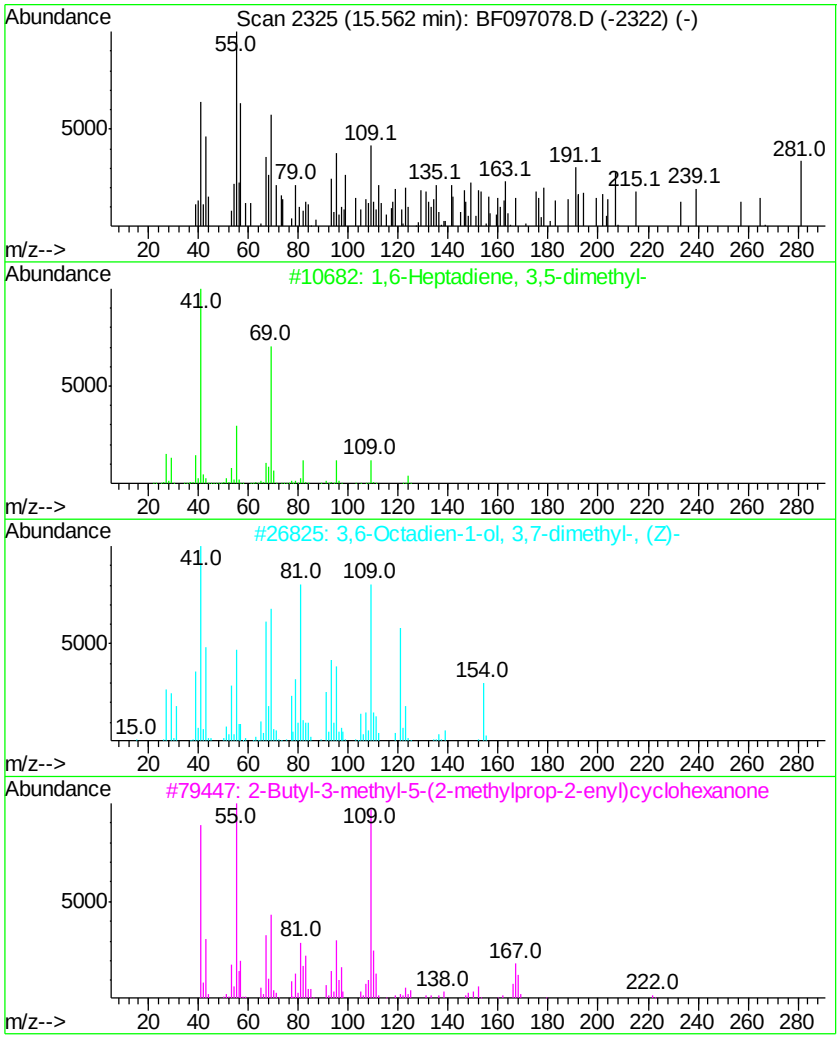
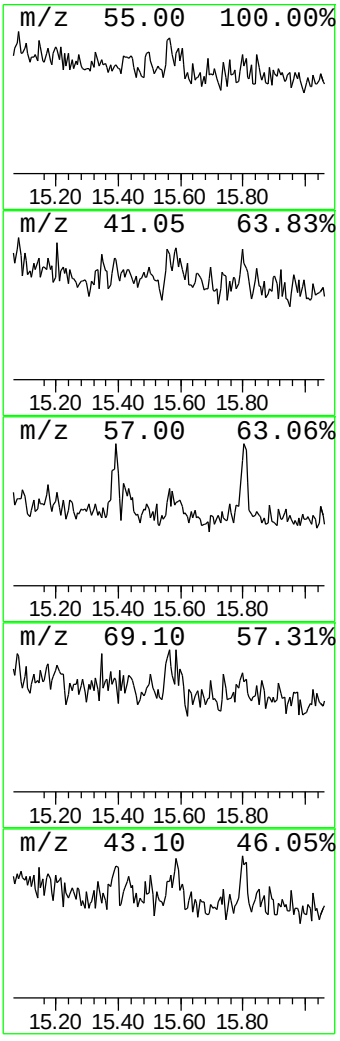
Peak Number 12 unknown15.56 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	2.14 ng	59072	Perylene-d12	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Heptadiene, 3,5-dimethyl-	124	C9H16	068701-99-5	11
2	3,6-Octadien-1-ol, 3,7-dimethyl-...	154	C10H18O	005944-20-7	10
3	2-Butyl-3-methyl-5-(2-methylprop...	222	C15H26O	1000281-10-7	10
4	1-Propene, 1,2-bis(difluorophosp...	178	C3H4F4P2	119280-18-1	9
5	4,7,7-Trimethylbicyclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097078.D
Acq On : 26 Jul 2017 16:37
Operator : SJ/JU
Sample : I4443-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E2-M7-NSW

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.65	9.5	ng	302838	1	6.49	639516	20.0
unknown11.50	11.50	3.0	ng	122434	4	11.00	822868	20.0
n-Hexadecanoic acid	11.56	2.4	ng	97642	4	11.00	822868	20.0
unknown11.75	11.75	4.2	ng	171101	4	11.00	822868	20.0
18-Norabietane	11.86	2.3	ng	94490	4	11.00	822868	20.0
unknown12.26	12.26	5.9	ng	243338	4	11.00	822868	20.0
unknown12.34	12.34	2.0	ng	51154	5	13.62	499434	20.0
Acridin-9-amine, ...	12.96	2.1	ng	53133	5	13.62	499434	20.0
Dichloroacetic ac...	13.50	5.2	ng	130037	5	13.62	499434	20.0
unknown13.93	13.93	3.1	ng	78474	5	13.62	499434	20.0
unknown15.56	15.56	2.1	ng	59072	6	14.97	551582	20.0