LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088130.D
Acq On : 18 Jun 2016 13:19
Operator : UM/SJ
Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

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-BF060716.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	1.667	4	7	15	rVB	166155	325116	13.68%	1.411%
2	1.781	15	17	25	rVV	1061242	1665599	70.08%	7.229%
3	1.884	25	26	41	rVB2	93931	238849	10.05%	1.037%
4	2.273	57	60	68	rVB	66758	104023	4.38%	0.451%
5	4.856	284	286	293	rBV	100724	182304	7.67%	0.791%
6	5.301	322	325	327	rBV	1541970	2227586	93.72%	9.668%
7	6.353	414	417	419	rBV	1853052	2237669	94.15%	9.712%
8	6.467	424	427	429	rVV	1876824	2376752	100.00%	10.315%
9	6.684	444	446	449	rBV	694195	579517	24.38%	2.515%
10	6.764	449	453	456	rBV	64248	70011	2.95%	0.304%
11	6.844	457	460	462	rVV	1916876	1878504	79.04%	8.153%
12	7.107	478	483	486	rBV2	14476	26551	1.12%	0.115%
13	7.256	493	496	498	rBV	1242412	1241202	52.22%	5.387%
14	7.644	528	530	534	rBV	24920	35144	1.48%	0.153%
15	7.736	534	538	541	rVV	20451	34100	1.43%	0.148%
16	7.976	556	559	561	rBV	602405	715171	30.09%	3.104%
17	8.753	625	627	631	rVB	50176	69001	2.90%	0.299%
18	8.947	642	644	645	rVB	22770	23876	1.00%	0.104%
19	8.982	645	647	650	rVB2	21219	24057	1.01%	0.104%
20	9.050	650	653	655	rBV	2225116	2089549	87.92%	9.069%
21	9.165	661	663	665	rVB	39118	36454	1.53%	0.158%
22	9.450	685	688	690	rBV	242350	211187	8.89%	0.917%
23	9.530	693	695	699	rVV	42557	73982	3.11%	0.321%
24	9.668	702	707	709	rBV	13629	24094	1.01%	0.105%
25	9.725	709	712	714	rVB	648796	697343	29.34%	3.027%
26	10.056	737	741	743	rBV3	13607	26656	1.12%	0.116%
27	10.159	749	750	754	rVB	31308	33697	1.42%	0.146%
28	10.376	764	769	771	rBV2	16408	31565	1.33%	0.137%
29	10.445	773	775	778	rBV3	39154	39331	1.65%	0.171%
30	10.513	778	781	783	rBV	912952	1128271	47.47%	4.897%
31	10.628	789	791	795	rBV	37391	62322	2.62%	0.270%
32	10.833	807	809	811	rBV	41942	52341	2.20%	0.227%
33	10.948	816	819	821	rVB	37506	64727	2.72%	0.281%
34	11.005	821	824	826	rVB2	17319	25942	1.09%	0.113%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088130.D
Acq On : 18 Jun 2016 13:19
Operator : UM/SJ
Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.073	829	830	835	rBV4	35299	76322	3.21%	0.331%
36	11.199	839	841	843	rBV	684338	589708	24.81%	2.559%
37	11.382	855	857	859	rVB2	22330	33194	1.40%	0.144%
38	11.439	859	862	864	rBV4	26486	52187	2.20%	0.226%
39	11.748	887	889	890	rBV	78943	85537	3.60%	0.371%
40	11.771	890	891	892	rVV	90777	70331	2.96%	0.305%
41	12.251	931	933	935	rBV	57944	95177	4.00%	0.413%
42	12.674	968	970	974	rBV	303250	325614	13.70%	1.413%
43	12.788	977	980	982	rBV	1464243	1486508	62.54%	6.452%
44	12.845	982	985	986	rVV	23022	38551	1.62%	0.167%
45	13.256	1019	1021	1024	rBV	194567	288840	12.15%	1.254%
46	13.828	1069	1071	1074	rBV2	524753	653933	27.51%	2.838%
47	14.285	1109	1111	1112	rBV	168284	173574	7.30%	0.753%
48	15.222	1190	1193	1196	rBV	308211	419021	17.63%	1.819%

Sum of corrected areas: 23040990

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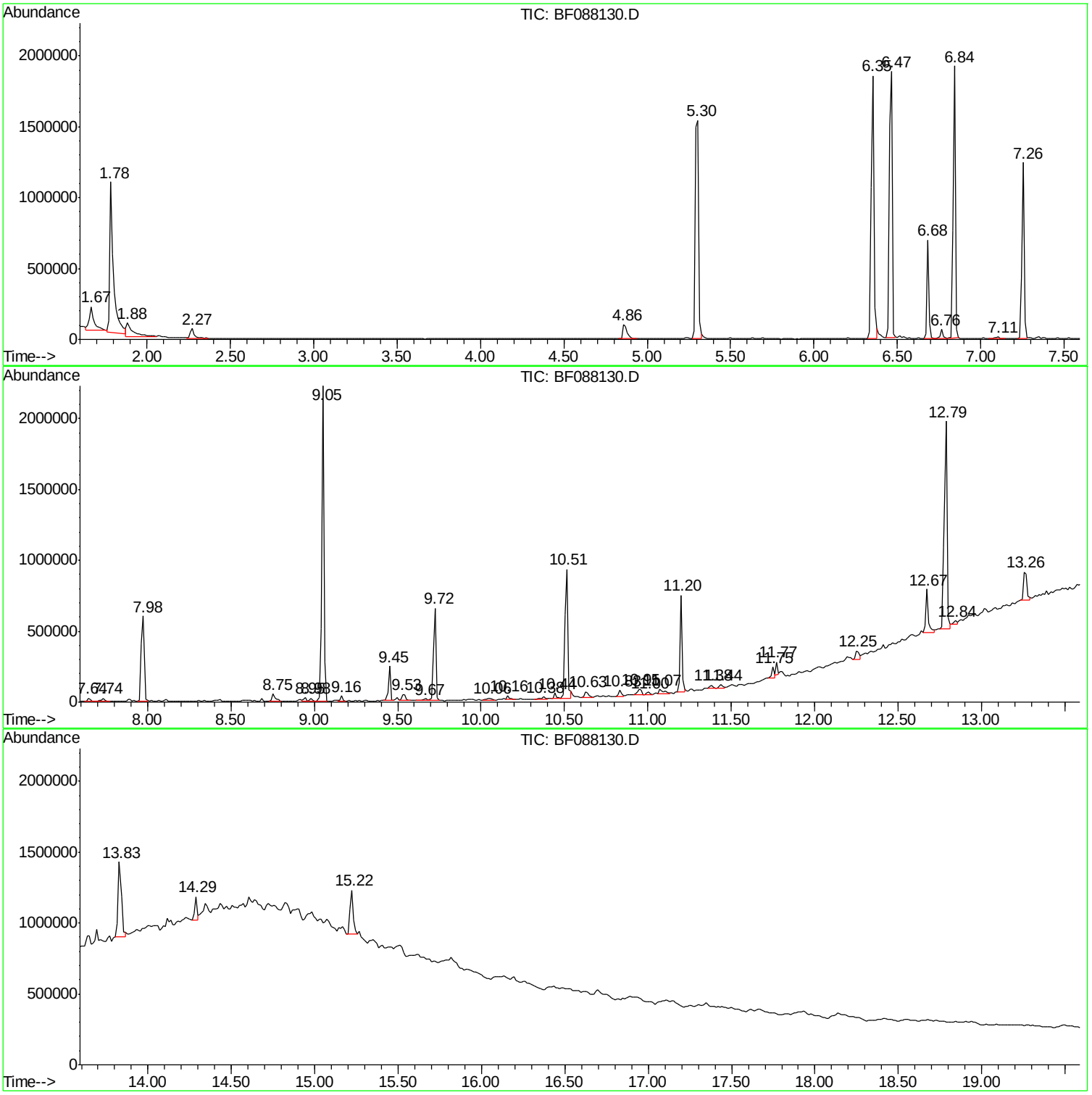
Instrument :
BNA_F
ClientSampleId :
SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061816\
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Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

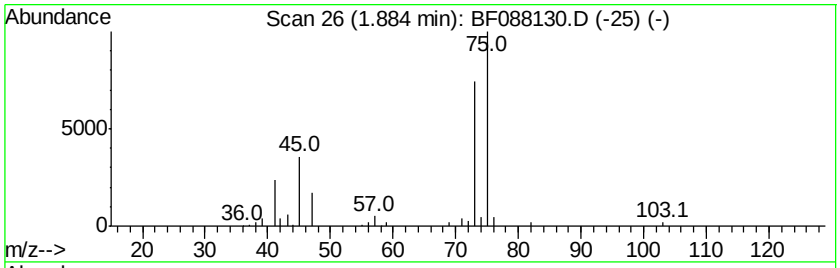
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

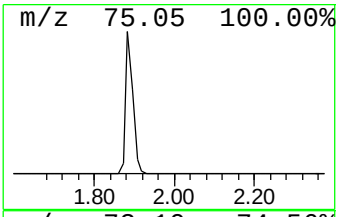
****

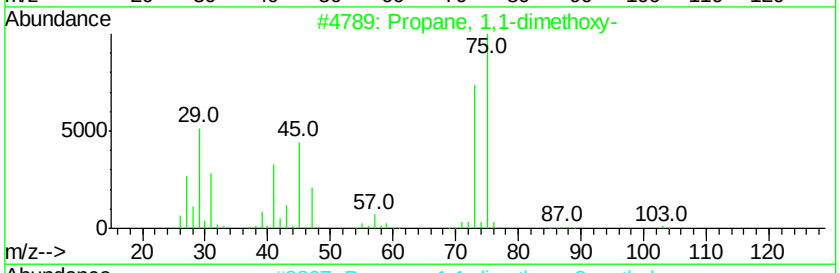
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

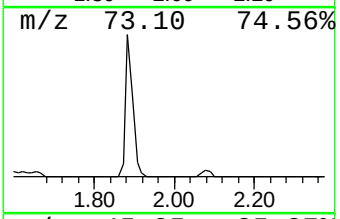
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	8.24 ng	238849	1,4-Dichlorobenzene-d4	6.68

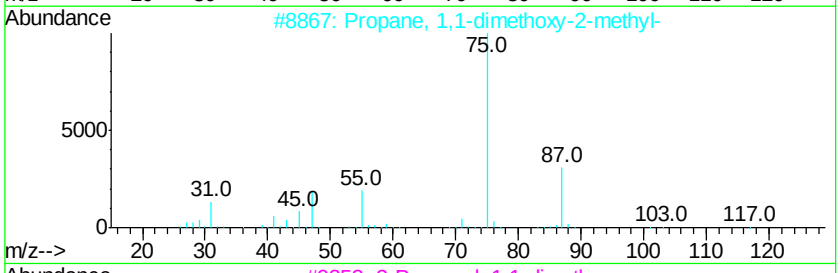
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	42
3	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5	Glycine	75	C2H5NO2	000056-40-6	9

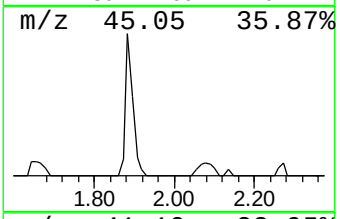


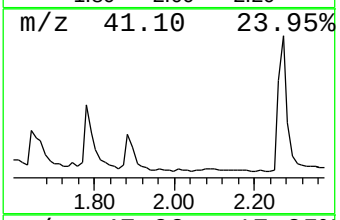


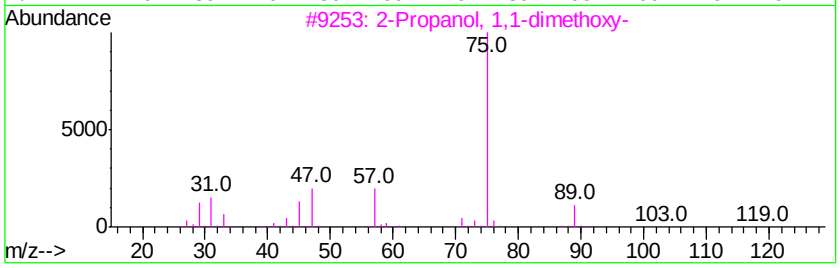


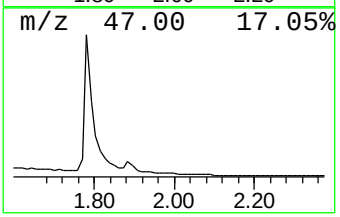












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Acq On : 18 Jun 2016 13:19
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Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

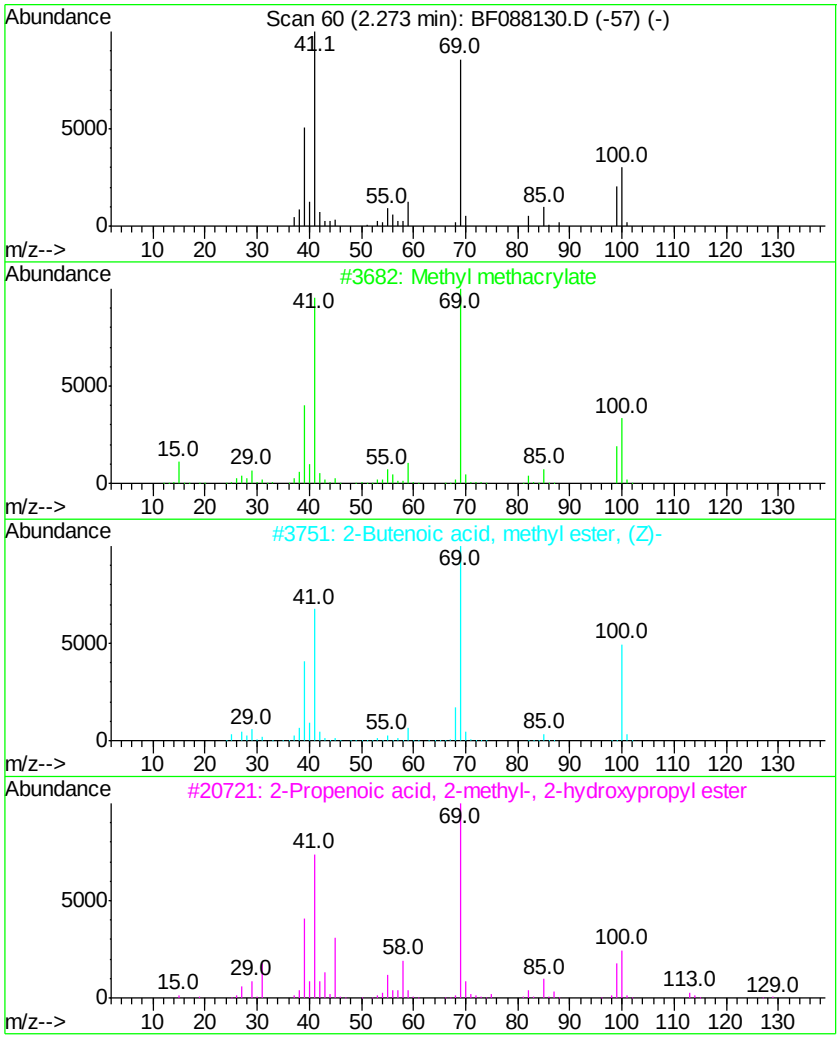
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

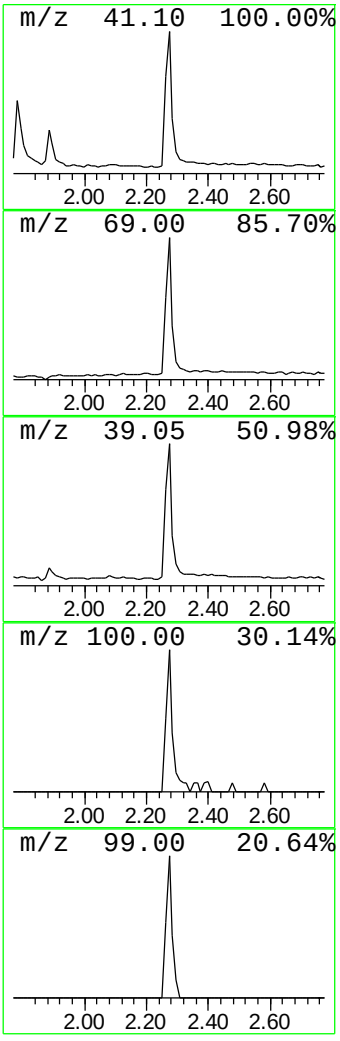
****

Peak Number 4 Methyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	3.59 ng	104023	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl methacrylate	100	C5H8O2	000080-62-6	95
2	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	83
3	2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	74
4	2-Butenoic acid, ethyl ester, (Z)-	114	C6H10O2	006776-19-8	59
5	Crotonyl isothiocyanate	127	C5H5NOS	060034-28-8	53





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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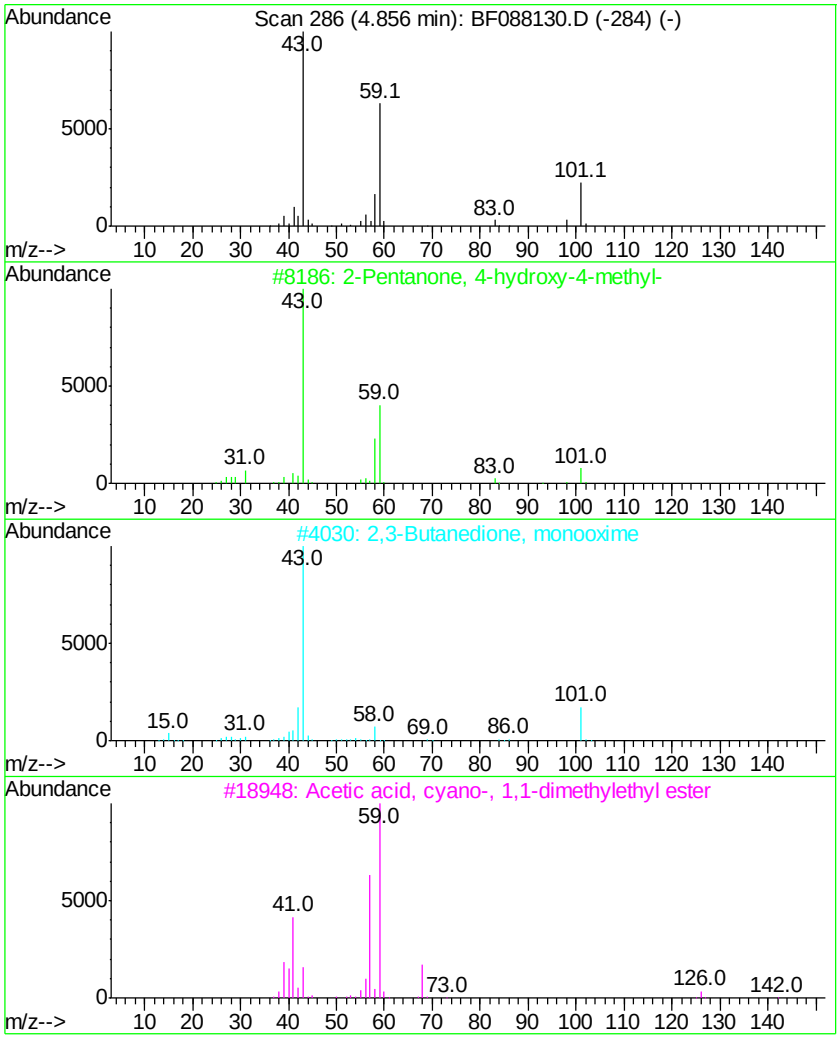
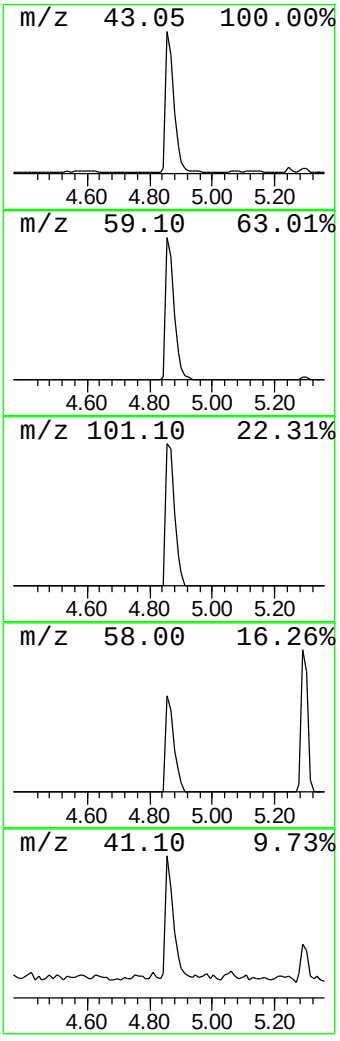
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	6.29 ng	182304	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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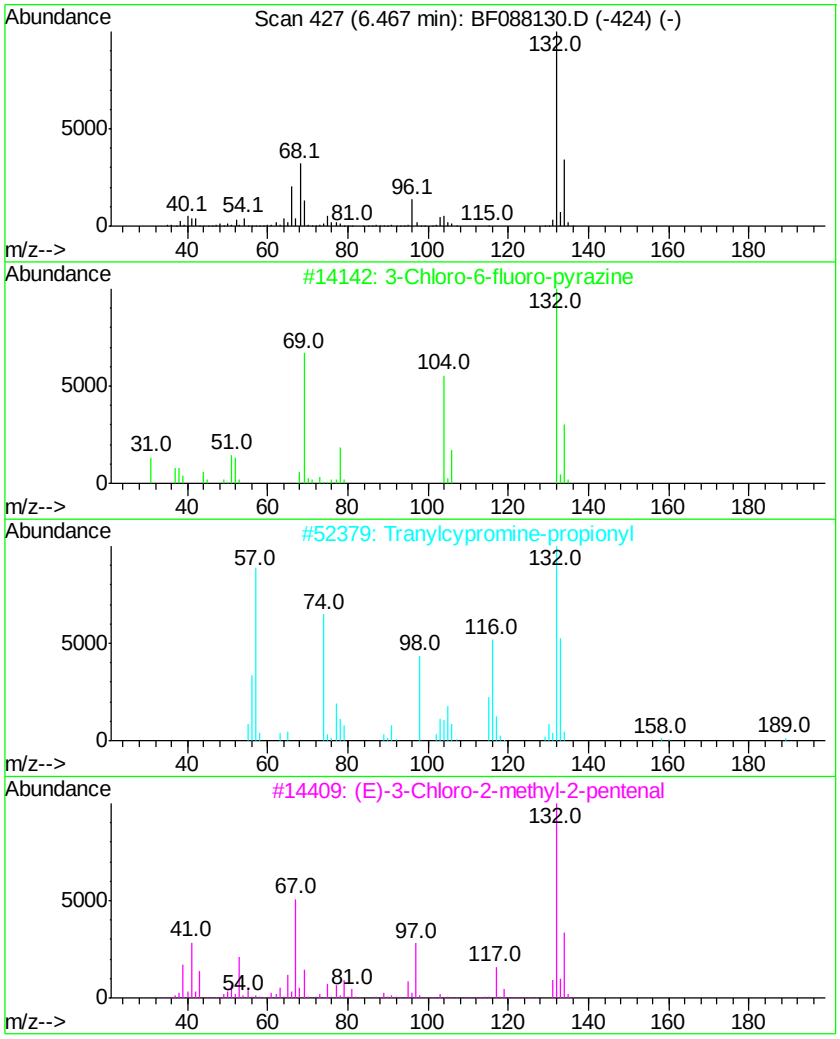
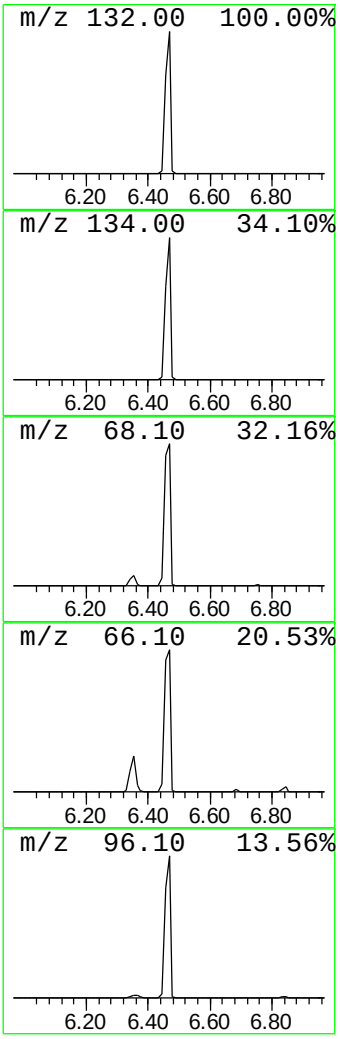
****

Peak Number 6 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	82.03 ng	2376750	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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

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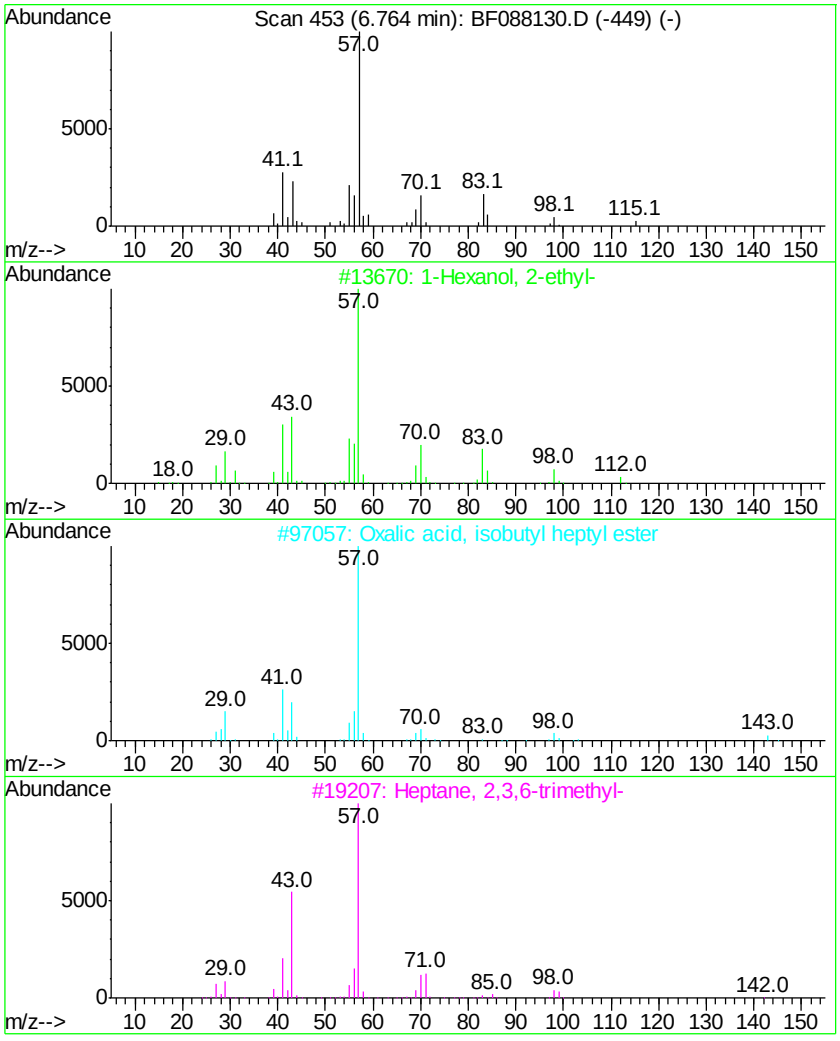
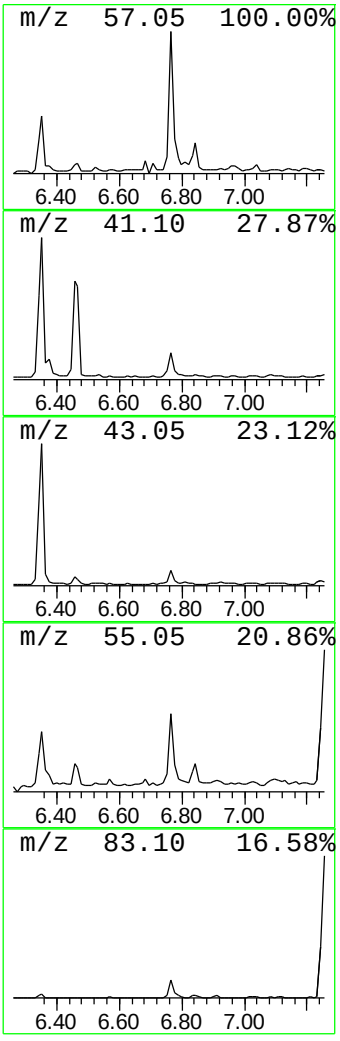
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	2.42 ng	70011	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	50
3	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	45
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	45
5	Heptane, 2-bromo-	178	C7H15Br	001974-04-5	43





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TIC Library : C:\Database\NIST11.L
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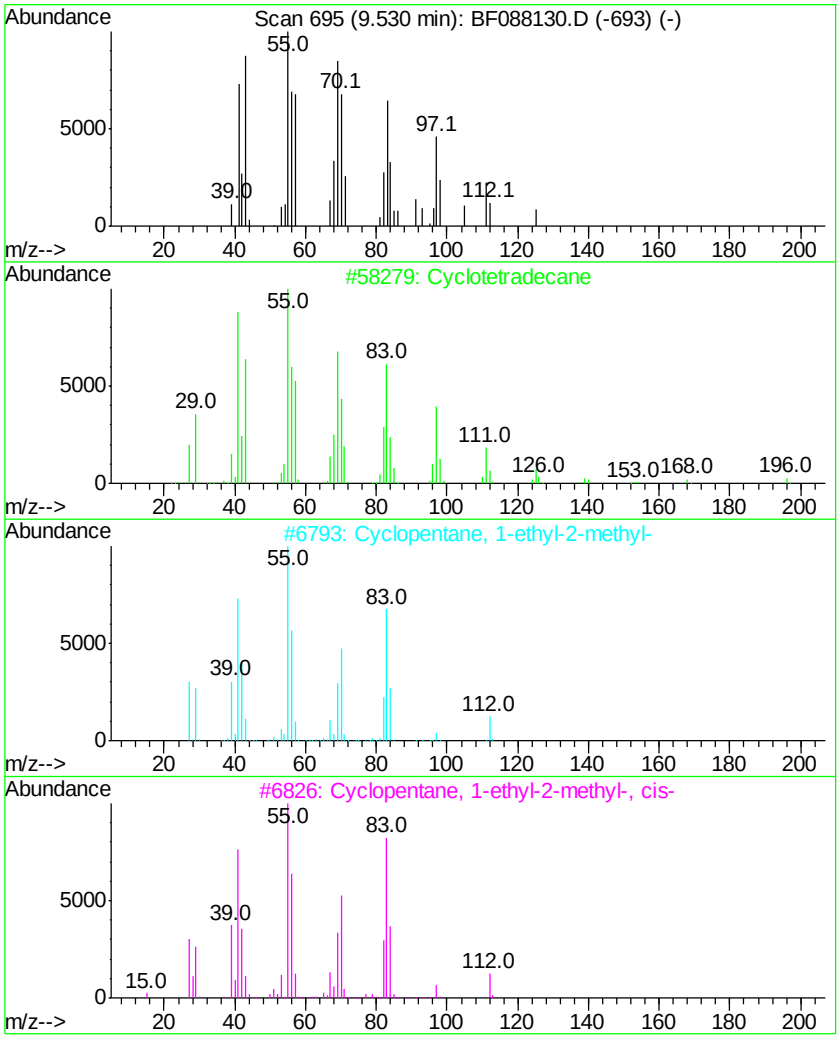
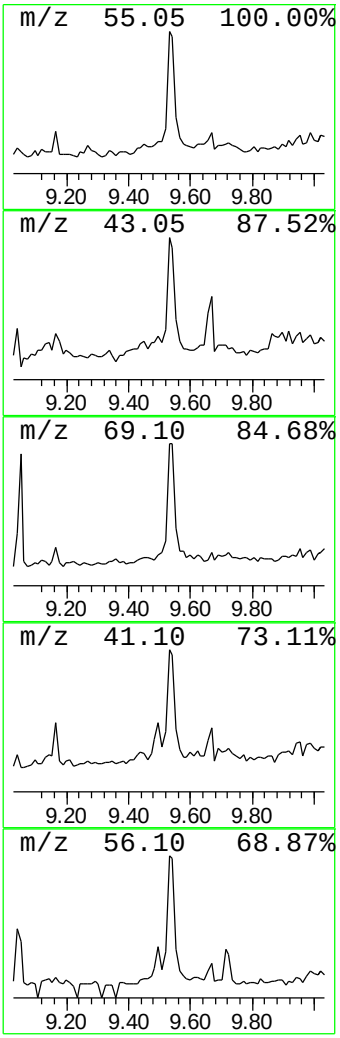
Peak Number 9 Cyclotetradecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	2.12 ng	73982	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	58
2	Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	50
3	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	46
4	Cyclooctane	112	C8H16	000292-64-8	43
5	Cycloheptane	98	C7H14	000291-64-5	41





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088130.D
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Operator : UM/SJ
Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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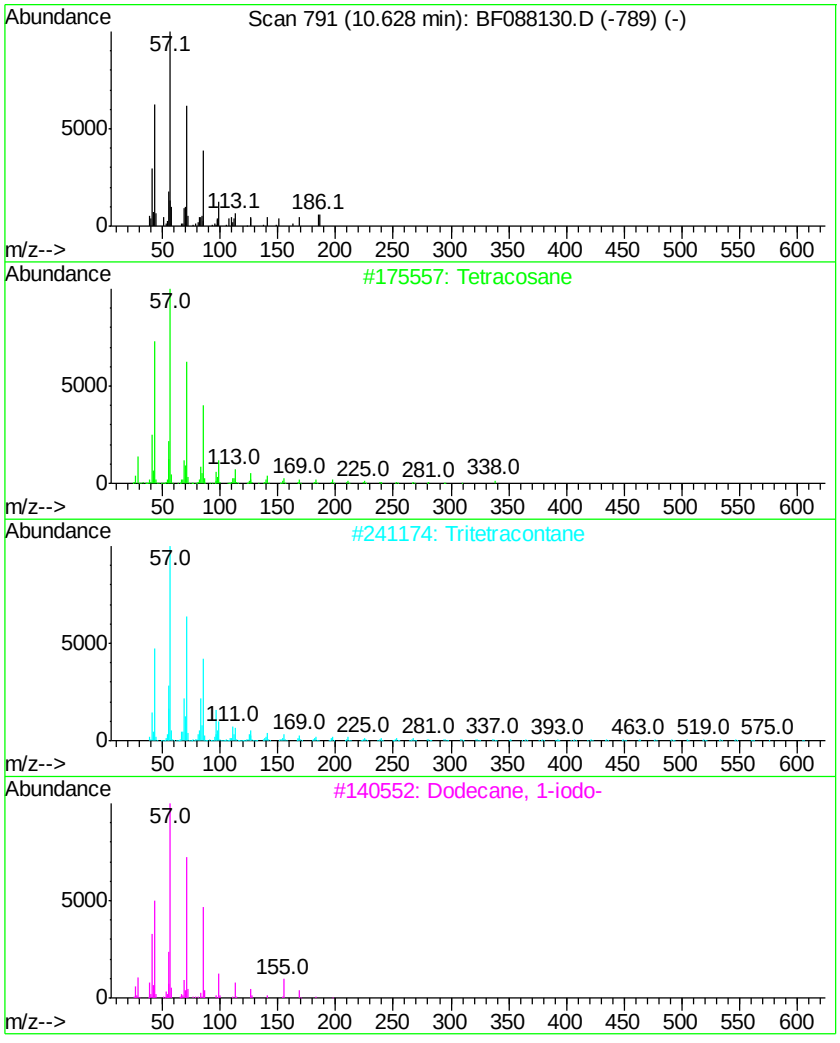
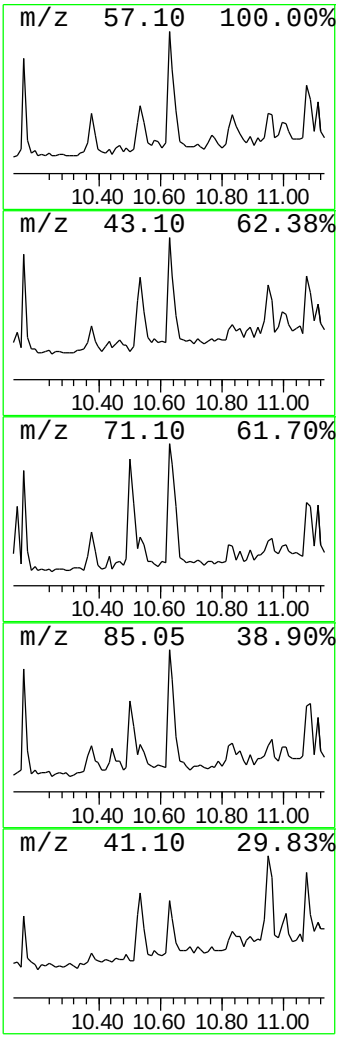
Peak Number 10 Tetracosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.11 ng	62322	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	83
2	Tritetracontane	605	C43H88	007098-21-7	80
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Tetratetracontane	619	C44H90	007098-22-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088130.D
Acq On : 18 Jun 2016 13:19
Operator : UM/SJ
Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

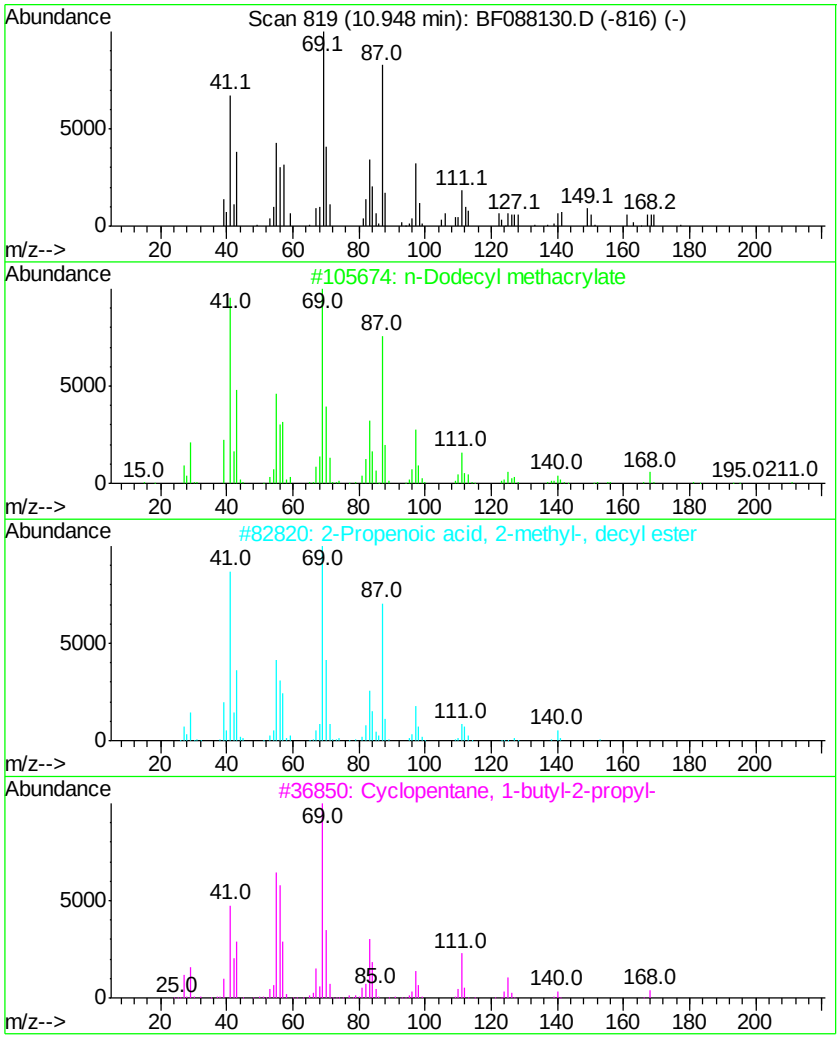
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

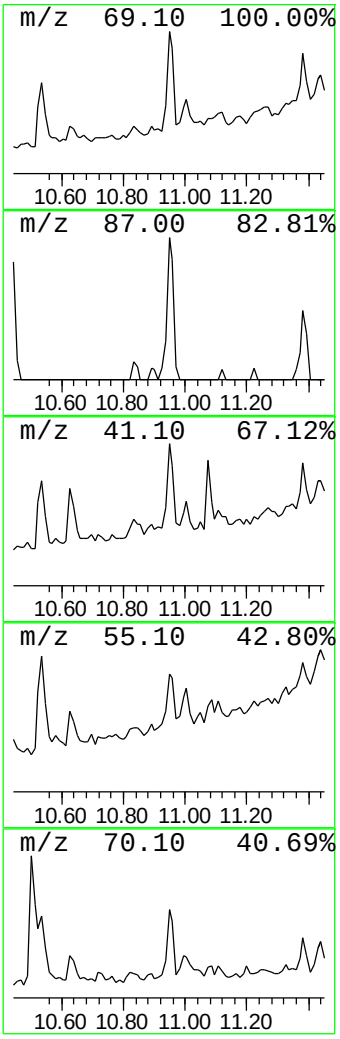
****

Peak Number 11 n-Dodecyl methacrylate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.20 ng	64727	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	86
3	Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	49
4	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	41
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088130.D
Acq On : 18 Jun 2016 13:19
Operator : UM/SJ
Sample : H3501-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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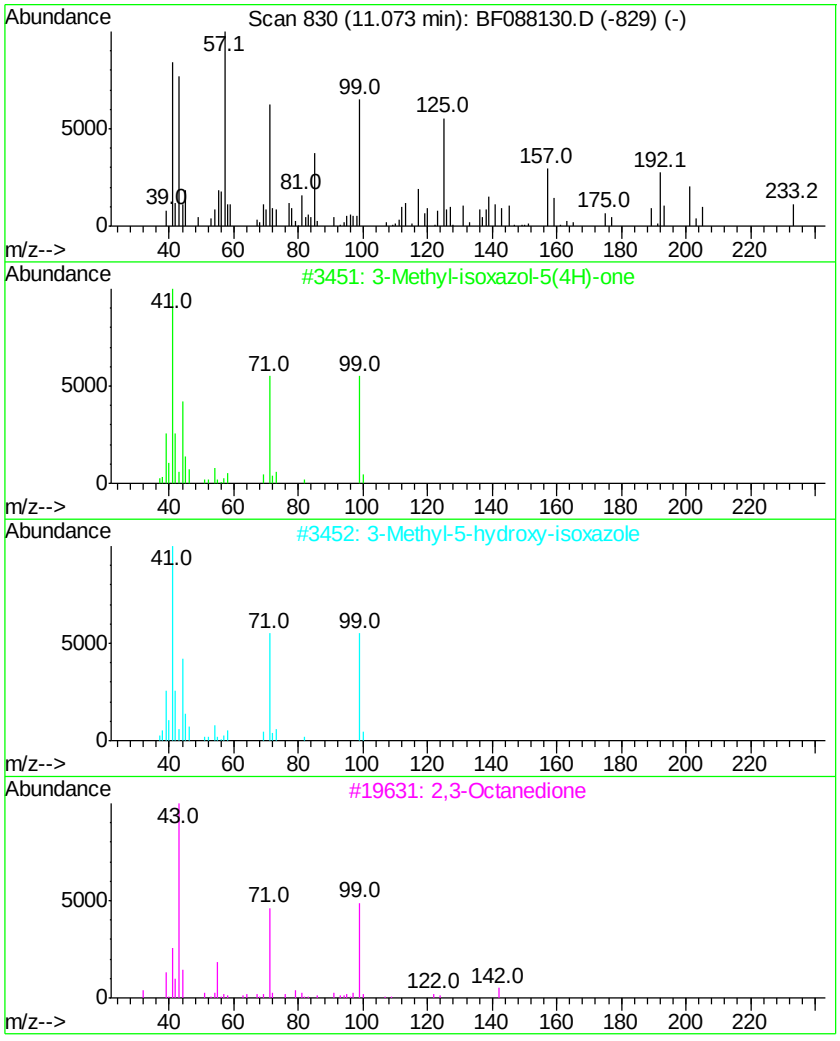
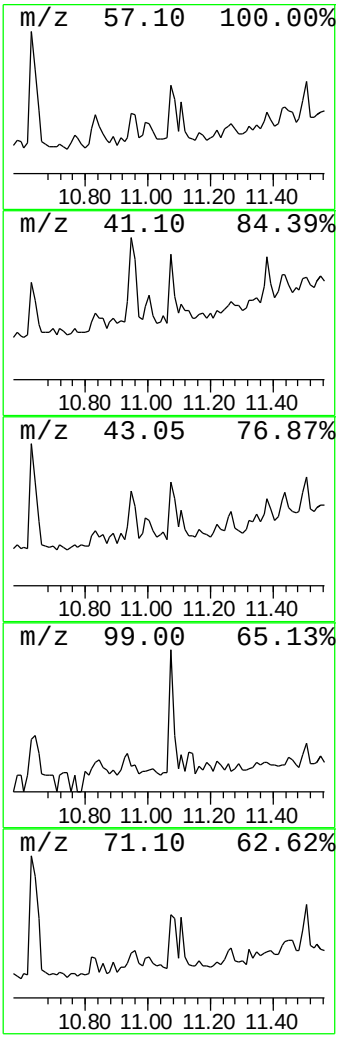
Peak Number 12 unknown11.07 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.07	2.59 ng	76322	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-isoxazol-5(4H)-one	99	C4H5NO2	001517-96-0	25
2	3-Methyl-5-hydroxy-isoxazole	99	C4H5NO2	045469-93-0	25
3	2,3-Octanedione	142	C8H14O2	000585-25-1	22
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	18
5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	14





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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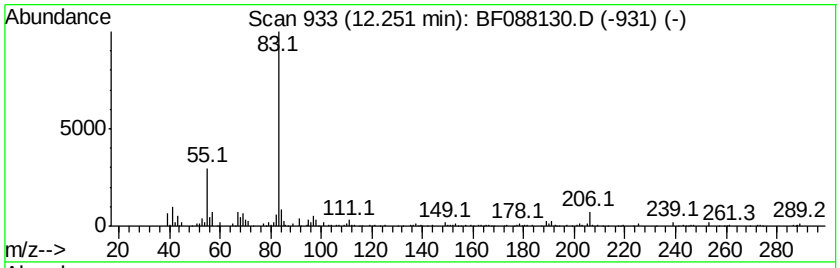
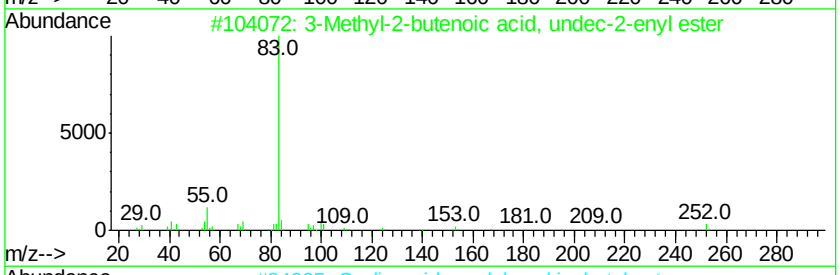
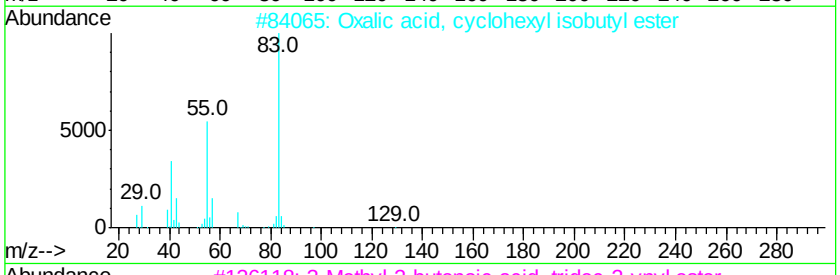
Peak Number 13 3-Methyl-2-butenoic acid, u... Concentration Rank 10

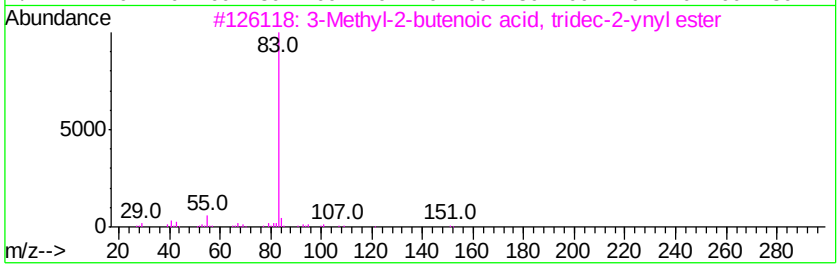
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	3.23 ng	95177	Phenanthrene-d10	11.20

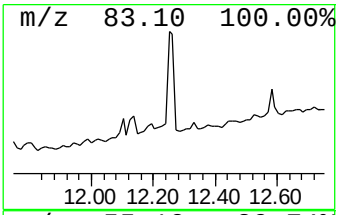
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-2-butenoic acid, undec-...	252	C16H28O2	1000299-31-6	64
2	Oxalic acid, cyclohexyl isobutyl...	228	C12H20O4	1000309-30-4	59
3	3-Methyl-2-butenoic acid, tridec...	278	C18H30O2	1000299-31-7	59
4	Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	59
5	Didecyl phosphite	362	C20H43O3P	007000-66-0	59

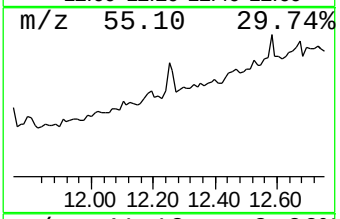


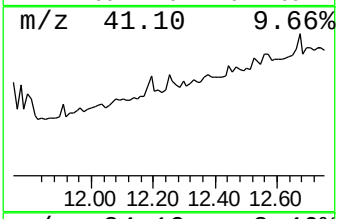


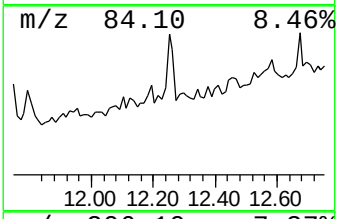


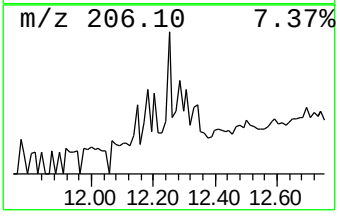












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Instrument : BNA_F
ClientSampleId : SS3-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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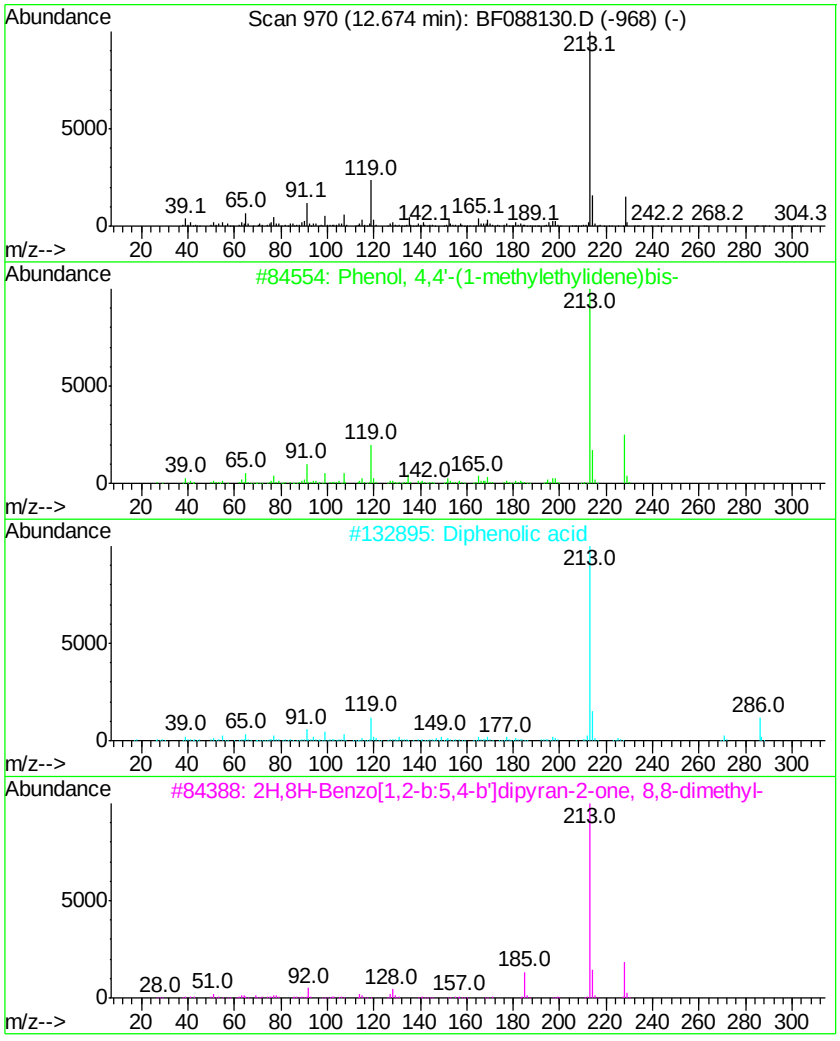
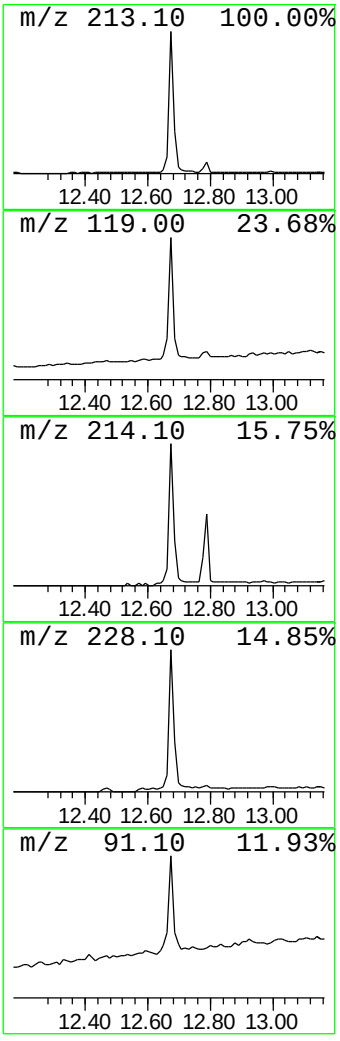
Peak Number 14 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	9.96 ng	325614	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	Diphenolic acid	286	C17H18O4	000126-00-1	56
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	52
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52





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TIC Integration Parameters: LSCINT.P

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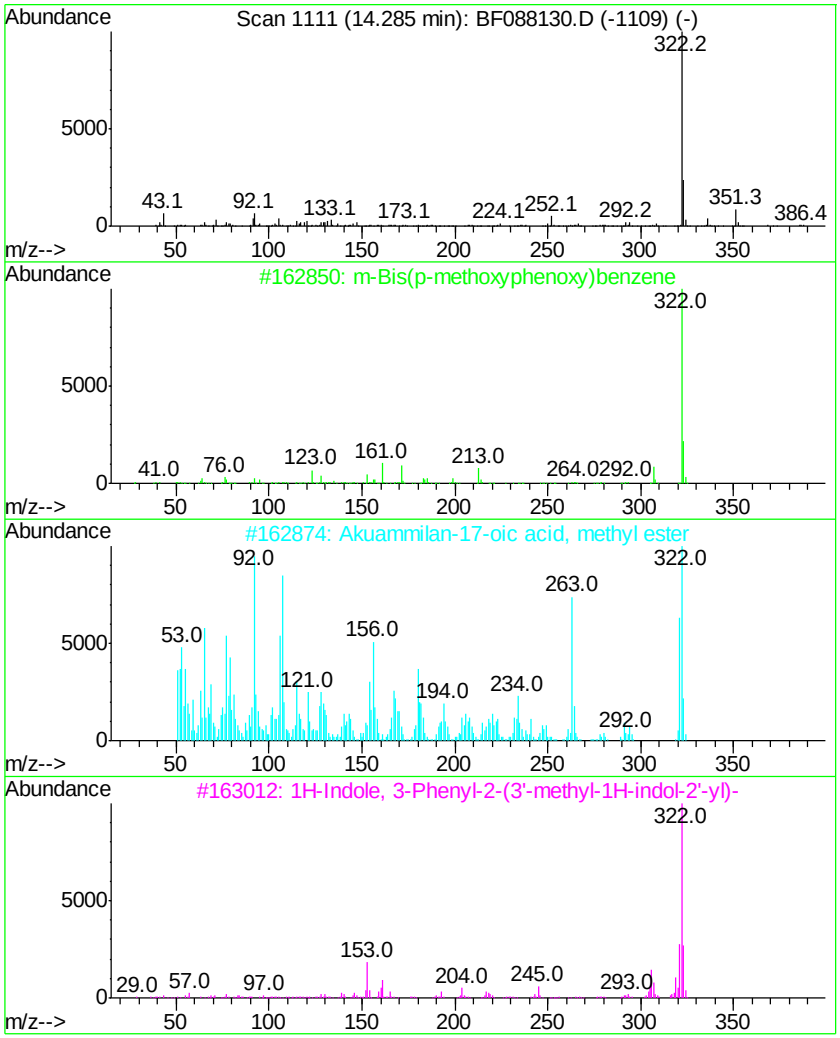
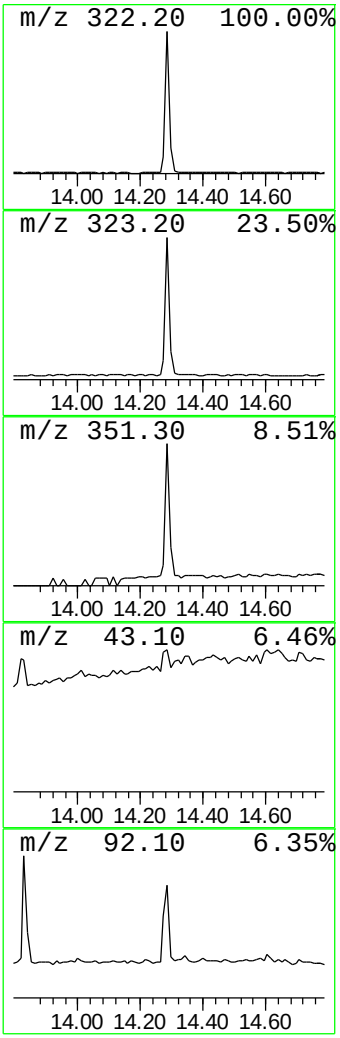
Peak Number 15 m-Bis(p-methoxyphenoxy)benzene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	5.31 ng	173574	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Bis(p-methoxyphenoxy)benzene	322	C20H18O4	013118-91-7	64
2	Akuammilan-17-oic acid, methyl e...	322	C20H22N2O2	006475-05-4	58
3	1H-Indole, 3-Phenyl-2-(3'-methyl...	322	C23H18N2	164936-86-1	56
4	Phenol, 2-(2H-benzotriazol-2-yl)...	351	C22H29N3O	025973-55-1	53
5	Pyrazole-4-carboxylic acid, 3-(1...	322	C20H22N2O2	1000272-86-5	39





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
Sample : H3501-03
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Instrument : BNA_F
ClientSampleId : SS3-0-6

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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
Propane, 1,1-dime...	1.88	8.2	ng	238849	1	6.68	579517	20.0
Methyl methacrylate	2.27	3.6	ng	104023	1	6.68	579517	20.0
2-Pentanone, 4-hy...	4.86	6.3	ng	182304	1	6.68	579517	20.0
unknown6.47	6.47	82.0	ng	2376750	1	6.68	579517	20.0
1-Hexanol, 2-ethyl-	6.76	2.4	ng	70011	1	6.68	579517	20.0
Cyclotetradecane	9.53	2.1	ng	73982	3	9.72	697343	20.0
Tetracosane	10.63	2.1	ng	62322	4	11.20	589708	20.0
n-Dodecyl methacr...	10.95	2.2	ng	64727	4	11.20	589708	20.0
unknown11.07	11.07	2.6	ng	76322	4	11.20	589708	20.0
3-Methyl-2-buteno...	12.25	3.2	ng	95177	4	11.20	589708	20.0
Phenol, 4,4'-(1-m...	12.67	10.0	ng	325614	5	13.83	653933	20.0
m-Bis(p-methoxyph...	14.29	5.3	ng	173574	5	13.83	653933	20.0