LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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	1.724	10	12	38	rVB	1302494	2605705	100.00%	38.182%
2	2.376	67	69	79	rVB	15700	34830	1.34%	0.510%
3	4.010	210	212	222	rBV	33286	65890	2.53%	0.965%
4	6.296	410	412	414	rBV	18002	38235	1.47%	0.560%
5	6.342	414	416	418	rVV	38112	55434	2.13%	0.812%
6	6.387	418	420	426	rVB	48479	96473	3.70%	1.414%
7	7.119	482	484	487	rBV	43555	74921	2.88%	1.098%
8	7.176	487	489	495	rVV2	43820	78923	3.03%	1.156%
9	7.313	498	501	510	rVB	23333	38459	1.48%	0.564%
10	7.885	549	551	555	rBV	204215	192882	7.40%	2.826%
11	8.445	598	600	604	rVB	34536	44493	1.71%	0.652%
12	8.959	641	645	647	rBV2	275684	412161	15.82%	6.039%
13	9.359	678	680	682	rBV	149343	150892	5.79%	2.211%
14	9.576	697	699	701	rVV2	22853	36421	1.40%	0.534%
15	9.633	701	704	706	rVB	306156	393450	15.10%	5.765%
16	9.896	725	727	729	rVV	19673	27761	1.07%	0.407%
17	10.022	735	738	741	rVV2	44165	64629	2.48%	0.947%
18	10.068	741	742	747	rVB	39253	47368	1.82%	0.694%
19	10.422	770	773	778	rVB2	151334	235408	9.03%	3.449%
20	10.536	781	783	787	rVB	38838	55008	2.11%	0.806%
21	10.719	797	799	801	rBV	29277	39834	1.53%	0.584%
22	10.982	820	822	824	rBV	32212	35521	1.36%	0.520%
23	11.108	831	833	835	rBV	421622	392918	15.08%	5.758%
24	11.657	878	881	888	rBV3	196525	235498	9.04%	3.451%
25	12.434	947	949	955	rVB	90532	115060	4.42%	1.686%
26	12.685	969	971	973	rBV	341066	315748	12.12%	4.627%
27	12.731	973	975	981	rVB	36471	45747	1.76%	0.670%
28	13.302	1023	1025	1029	rBV	59507	77929	2.99%	1.142%
29	13.417	1033	1035	1038	rVV	25058	38517	1.48%	0.564%
30	13.588	1048	1050	1055	rBV3	55040	108176	4.15%	1.585%
31	13.737	1060	1063	1065	rBV	309320	356183	13.67%	5.219%
32	13.805	1067	1069	1072	rVB2	34792	35431	1.36%	0.519%
33	15.097	1180	1182	1190	rVB	196727	278542	10.69%	4.082%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
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Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument :
BNA_F
ClientSampleId :
LF017MW001-160512

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

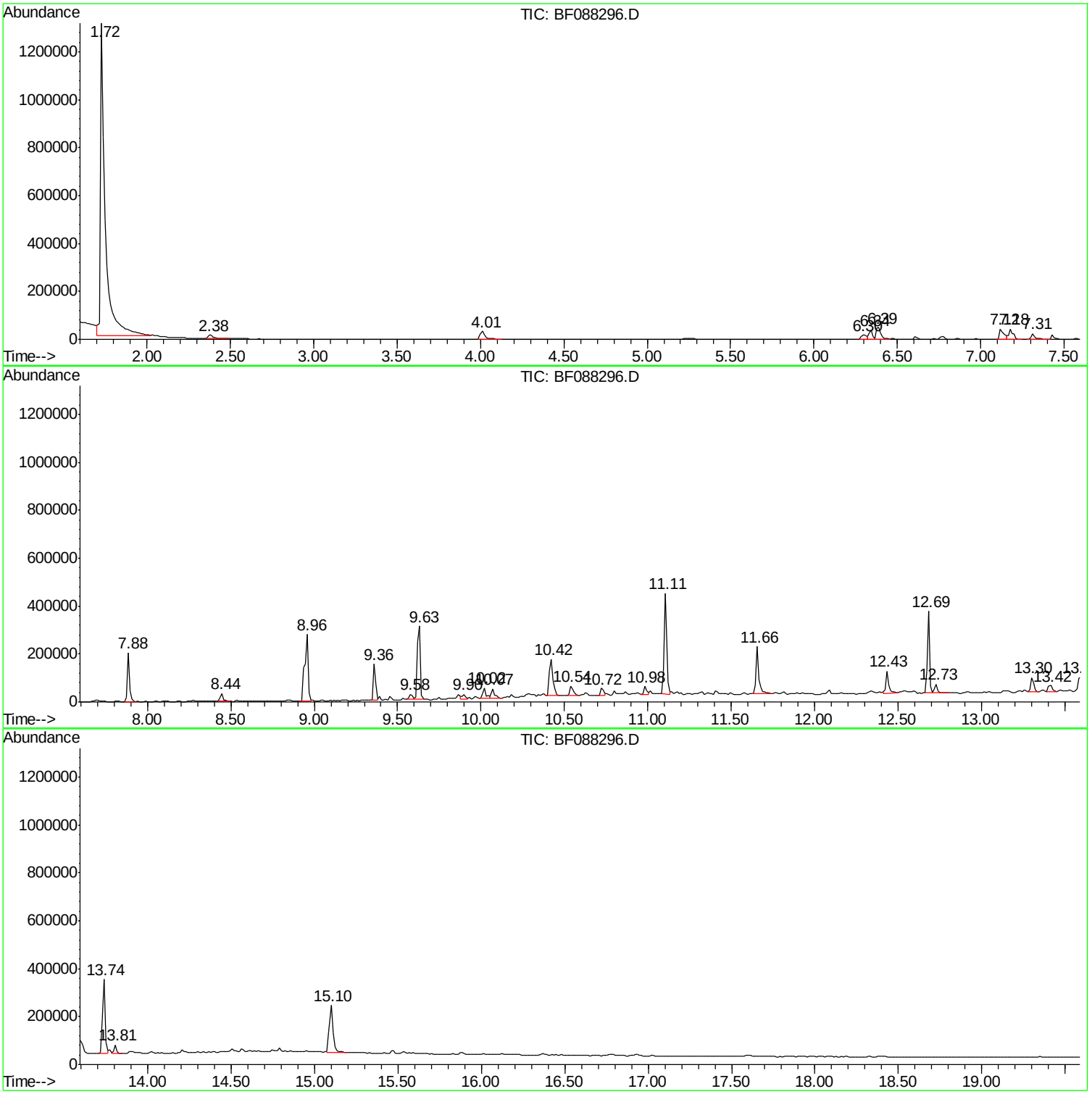
Sum of corrected areas: 6824447

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument :
BNA_F
ClientSampleId :
LF017MW001-160512

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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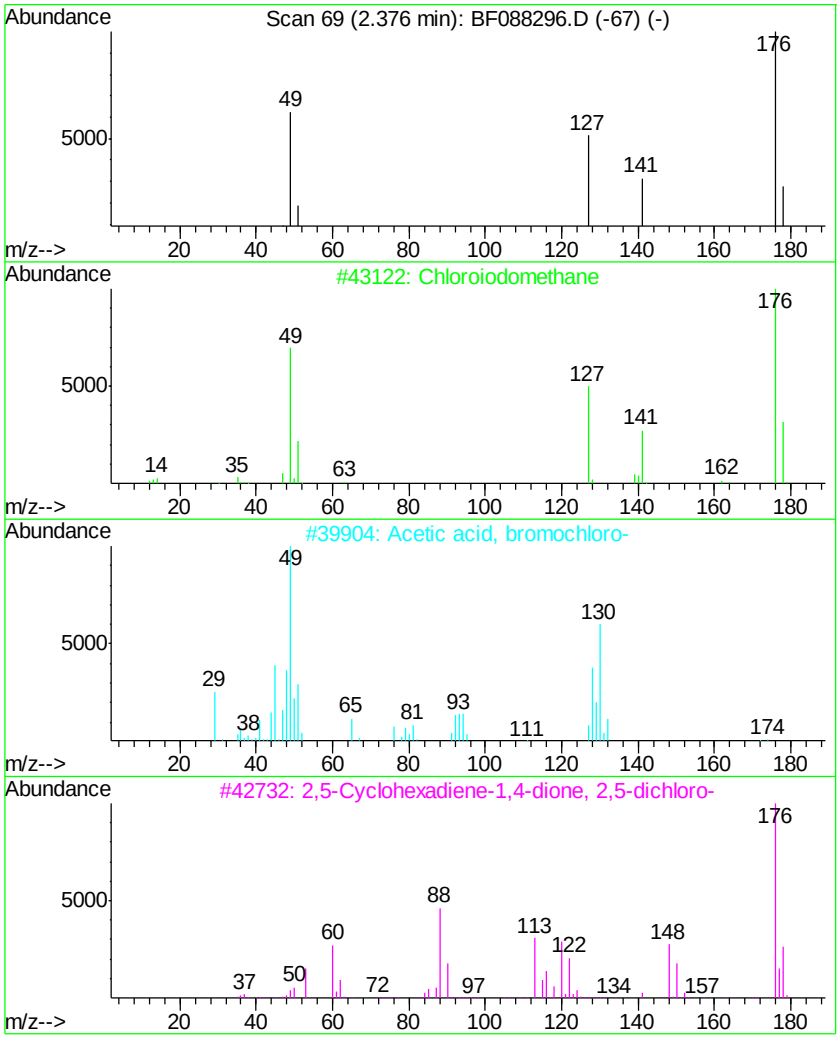
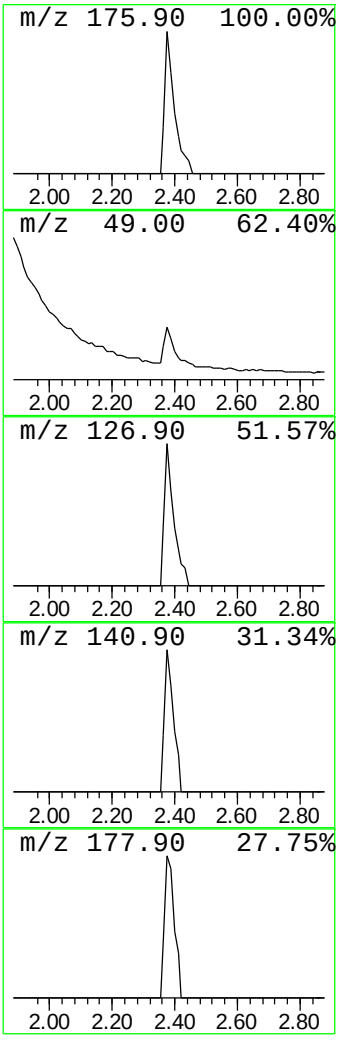
****

Peak Number 2 Chloroiodomethane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	1.81 ng	34830	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroiodomethane	176	CH2ClI	000593-71-5	91
2	Acetic acid, bromochloro-	172	C2H2BrClO2	005589-96-8	9
3	2,5-Cyclohexadiene-1,4-dione, 2,...	176	C6H2Cl2O2	000615-93-0	5
4	2-Methyl-1-nitroindolizine	176	C9H8N2O2	003243-10-5	4
5	3-Amino-7-methyl-1,2,4-benzotria...	176	C8H8N4O	027281-74-9	4





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
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Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

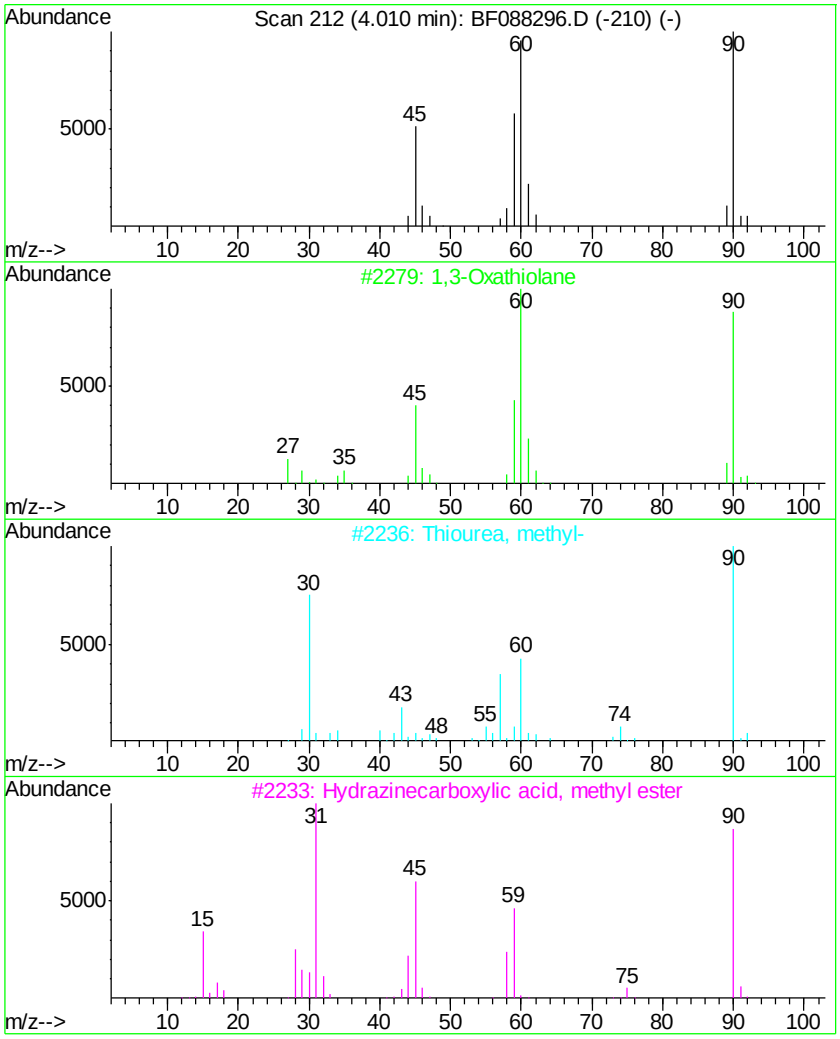
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

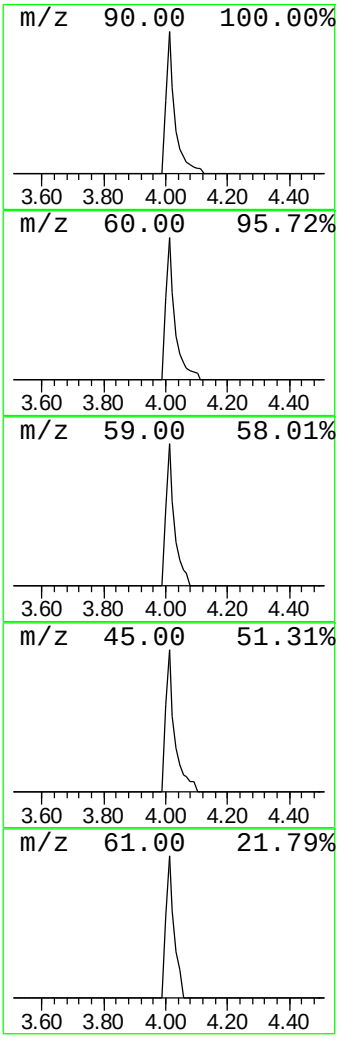
****

Peak Number 3 1,3-Oxathiolane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	3.41 ng	65890	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	96
2	Thiourea, methyl-	90	C2H6N2S	000598-52-7	64
3	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	59
4	3-Thietanol	90	C3H6OS	010304-16-2	42
5	Trisilane	92	H8Si3	007783-26-8	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
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Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

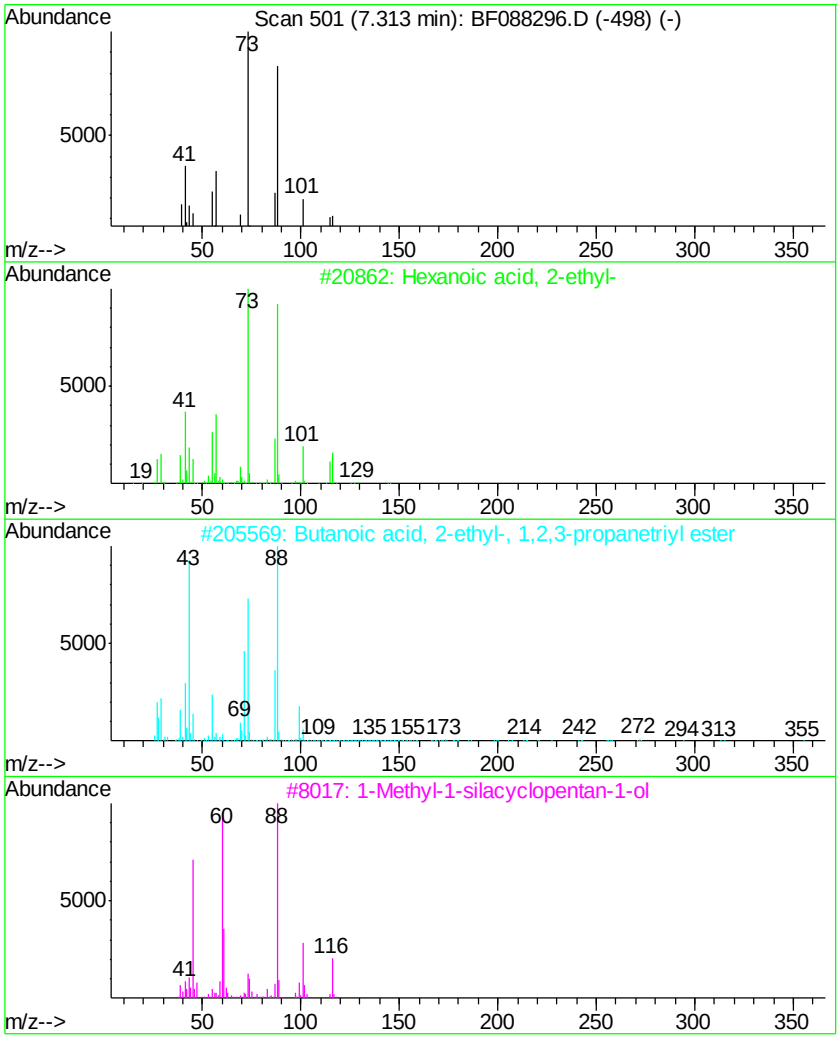
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

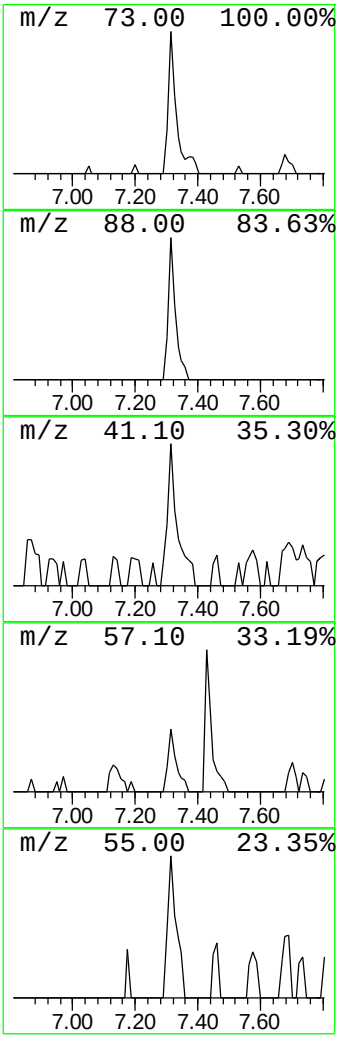
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	1.00 ng	38459	Naphthalene-d8	7.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	36
3	1-Methyl-1-silacyclopentan-1-ol	116	C5H12OSi	1000216-84-4	33
4	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	33
5	3-Hexanol, 3,5-dimethyl-	130	C8H18O	004209-91-0	12





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Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

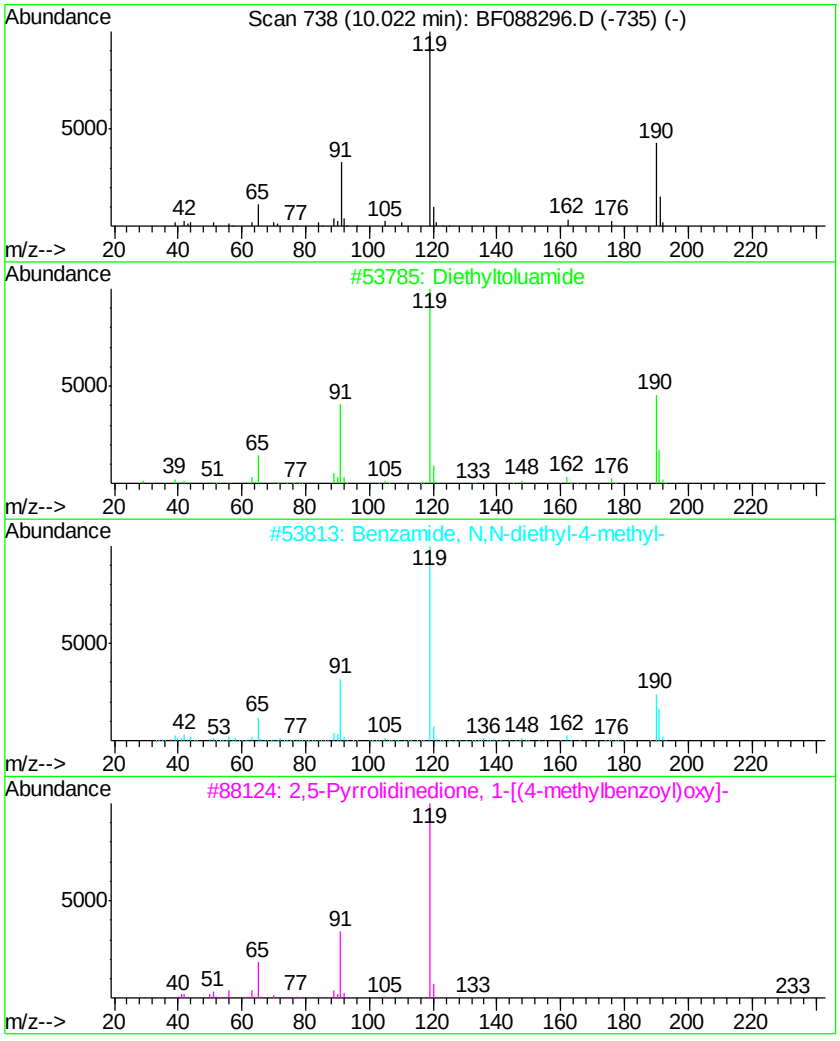
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

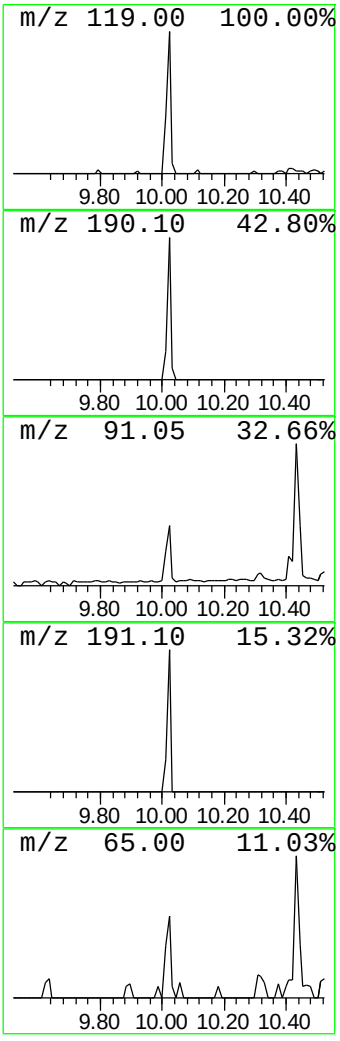
****

Peak Number 6 Diethyltoluamide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	0.82 ng	64629	Acenaphthene-d10	9.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	95
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3	2,5-Pyrrolidinedione, 1-[(4-meth...	233	C12H11NO4	083039-57-0	50
4	Benzamide, 2-chloro-5-(3-methylb...	288	C15H13ClN2O2	349489-17-4	50
5	Benzhydrazide, 4-methyl-N2-[1-me...	303	C12H13N7O3	324021-25-2	50





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Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

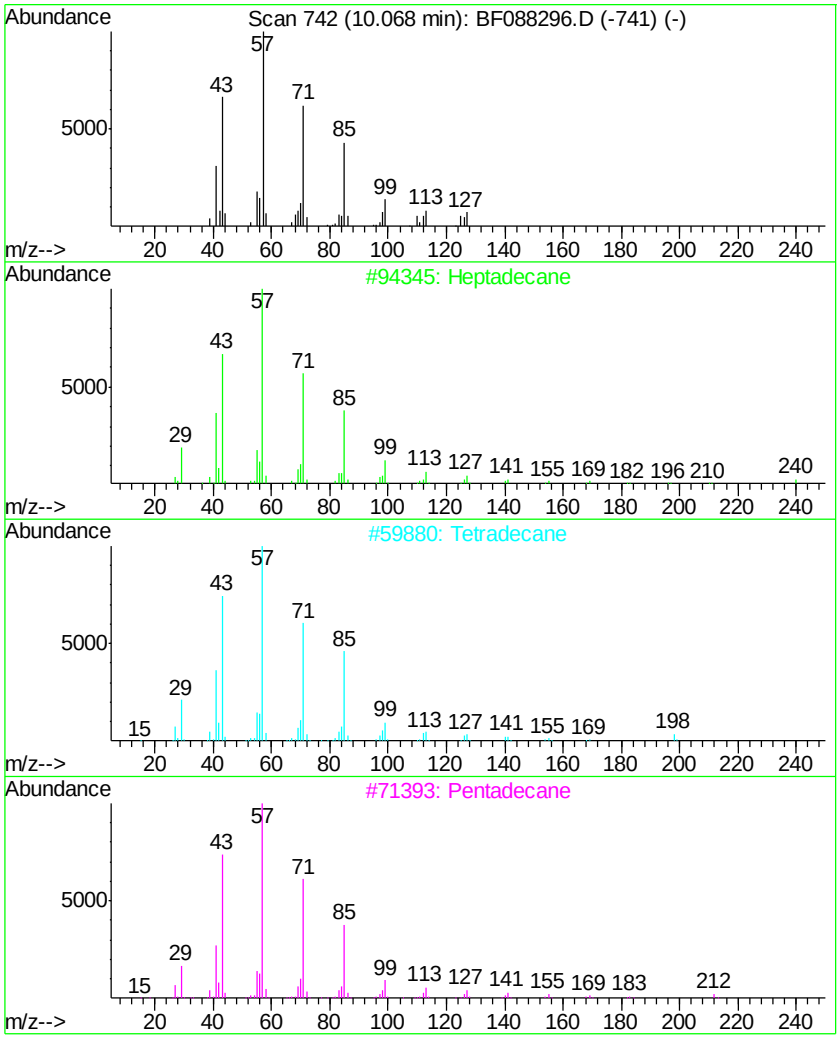
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

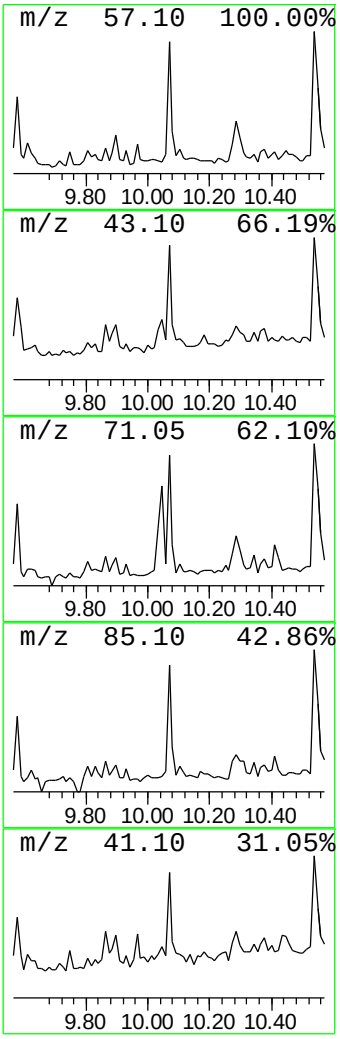
****

Peak Number 7 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	0.60 ng	47368	Acenaphthene-d10	9.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Tetradecane	198	C14H30	000629-59-4	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Hexadecane	226	C16H34	000544-76-3	78
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72





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Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

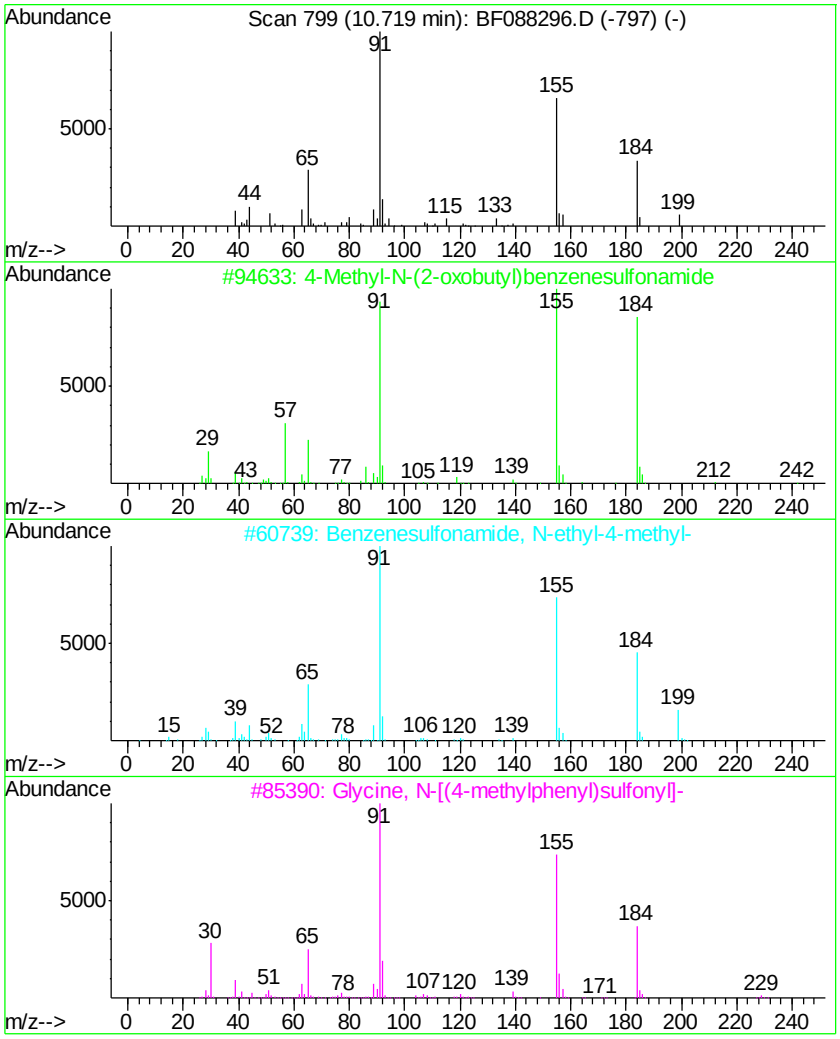
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

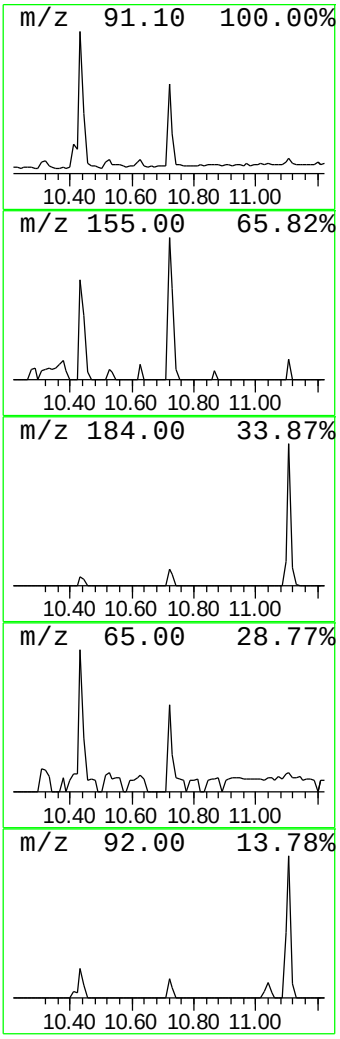
****

Peak Number 9 4-Methyl-N-(2-oxobutyl)benz... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	0.51 ng	39834	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	86
2	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	86
3	Glycine, N-[(4-methylphenyl)sulf...	229	C9H11NO4S	001080-44-0	64
4	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	59
5	(Toluene-4-sulfonylamino)-acetic...	283	C13H17NO4S	1000190-48-0	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
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Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

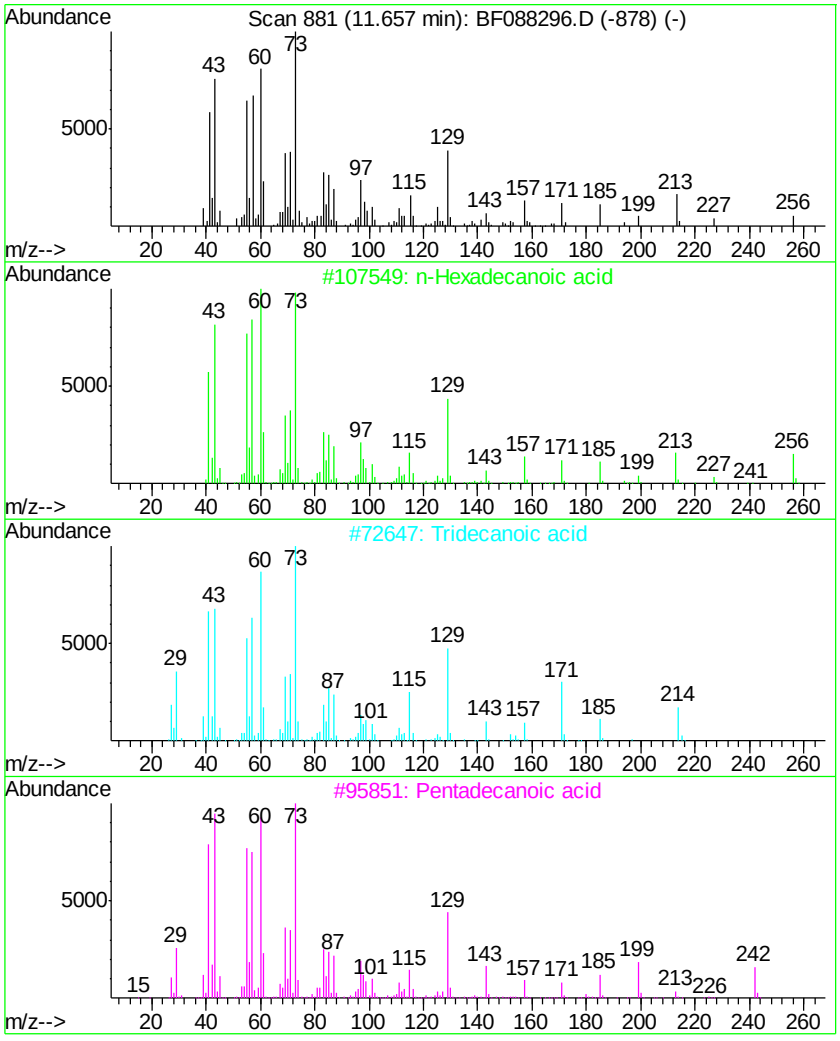
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

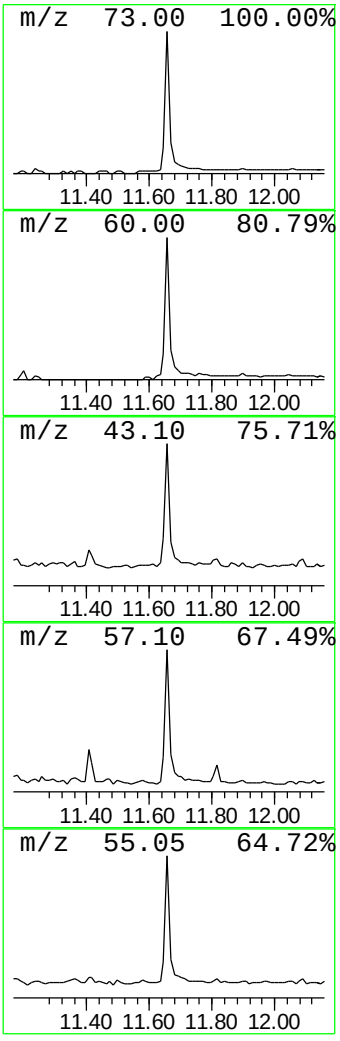
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.00 ng	235498	Phenanthrene-d10	11.11

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

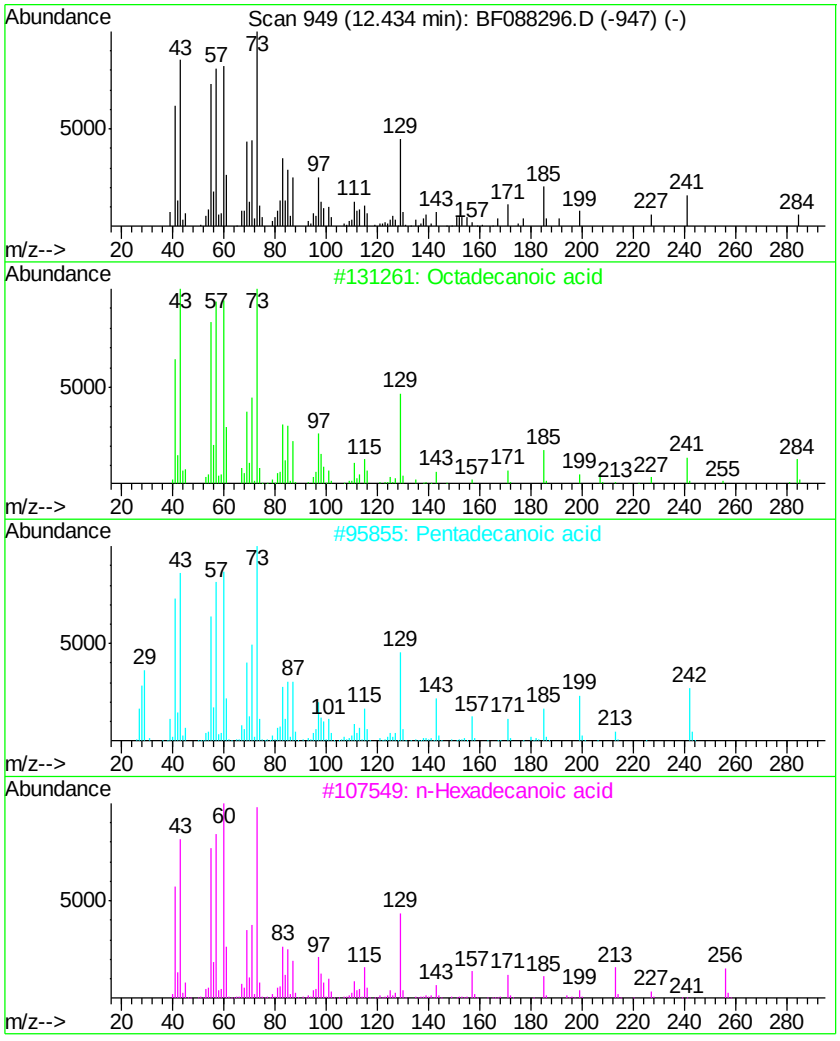
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

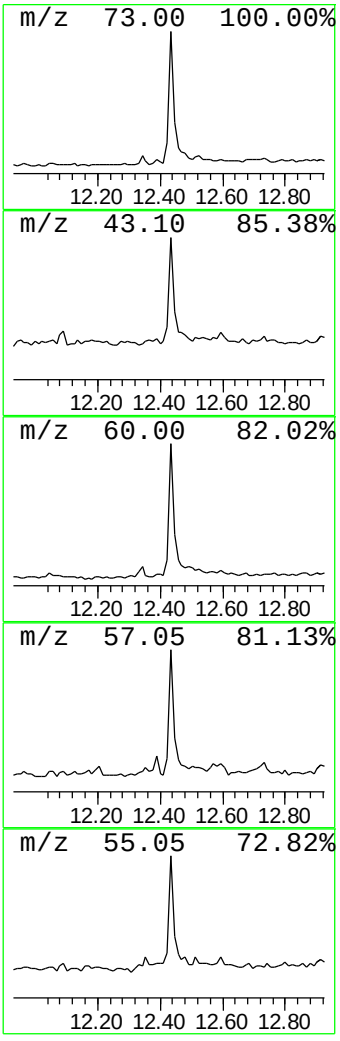
****

Peak Number 11 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	1.62 ng	115060	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	18





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

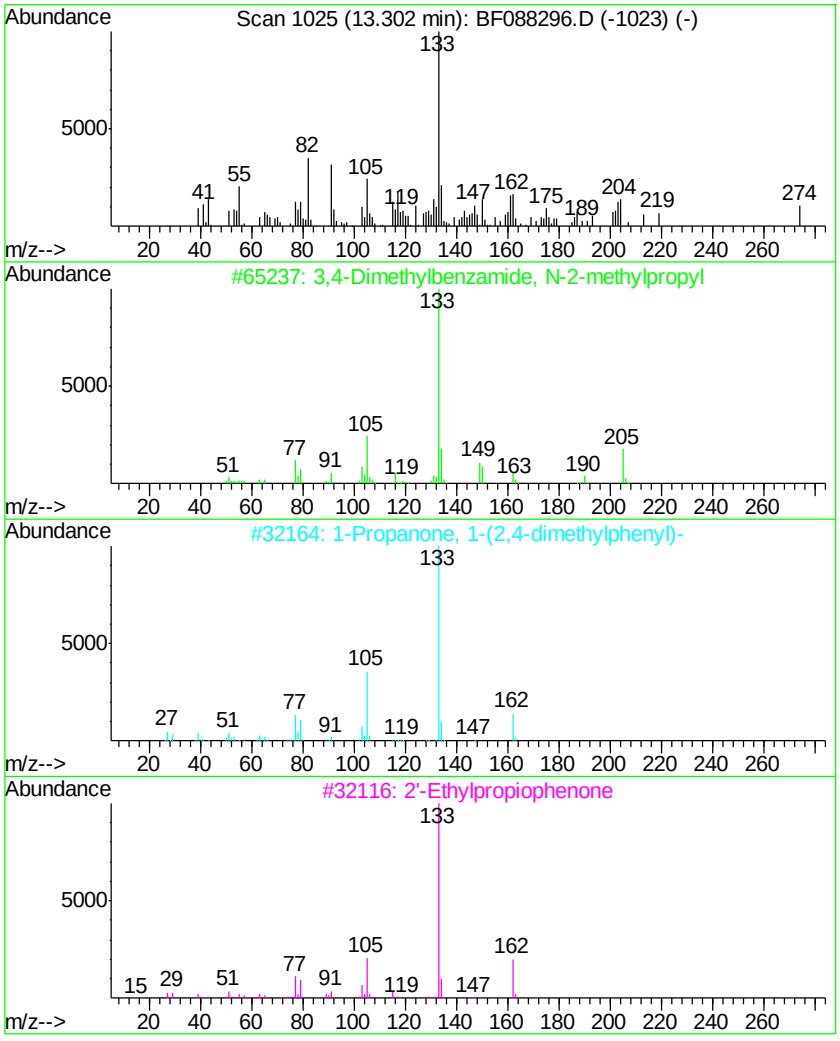
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

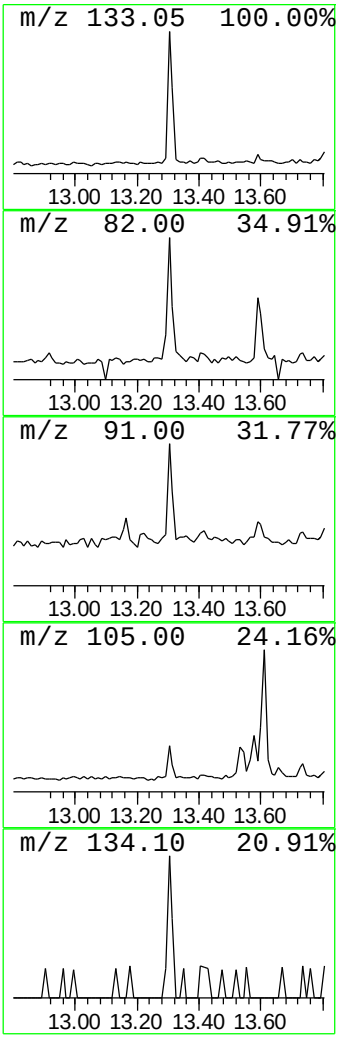
****

Peak Number 12 3,4-Dimethylbenzamide, N-2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	1.09 ng	77929	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylbenzamide, N-2-methy...	205	C13H19NO	333348-22-4	50
2	1-Propanone, 1-(2,4-dimethylphen...	162	C11H14O	035031-55-1	46
3	2'-Ethylpropiophenone	162	C11H14O	016819-79-7	46
4	4-Indolyl acetate	175	C10H9NO2	005585-96-6	43
5	Benzoic acid, 3,4-dimethyl-, eth...	178	C11H14O2	033499-44-4	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

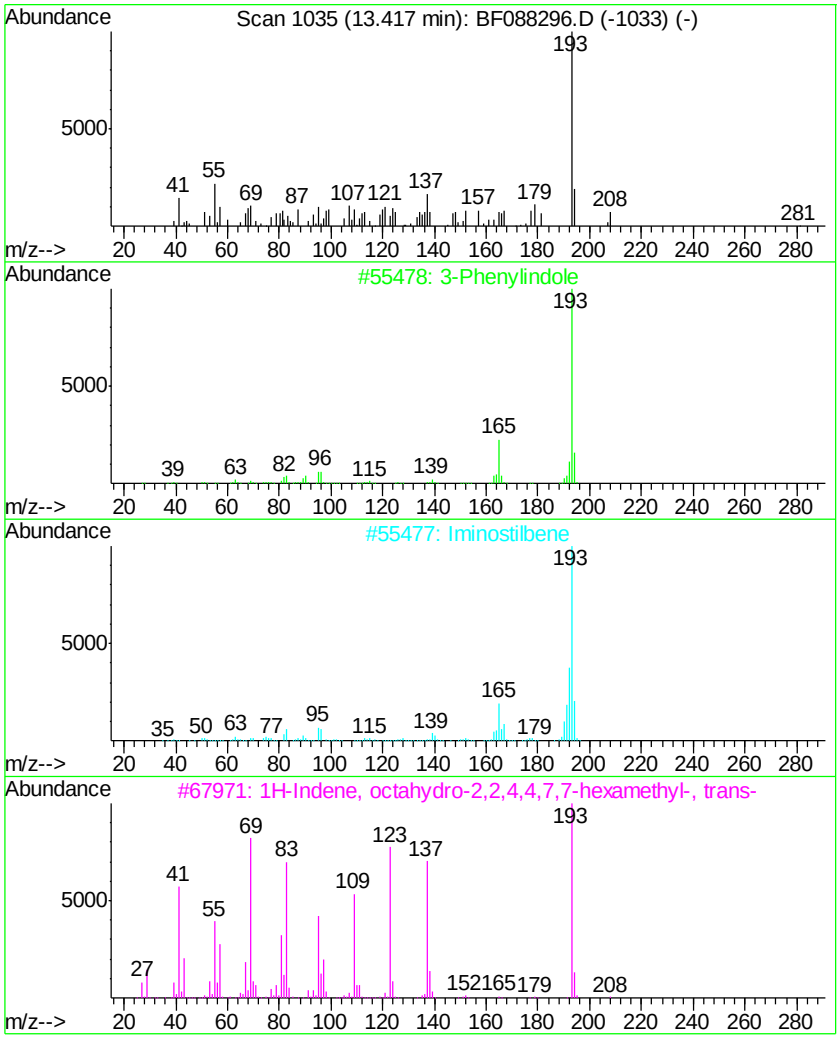
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

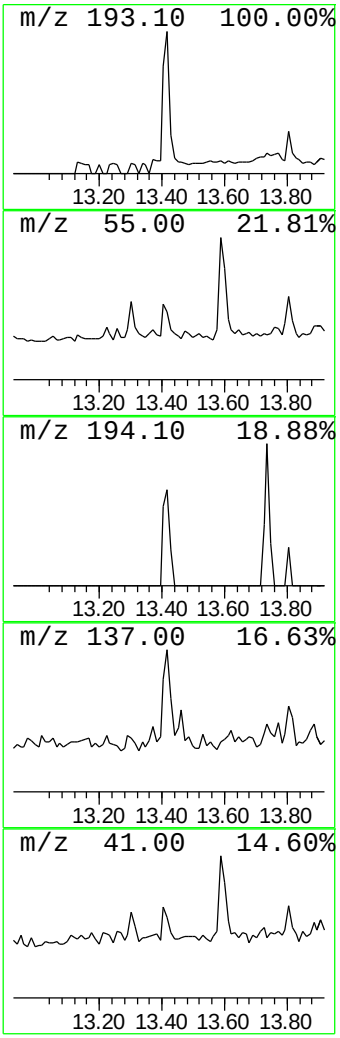
****

Peak Number 13 3-Phenylindole Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	0.54 ng	38517	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylindole	193	C14H11N	001504-16-1	50
2	Iminostilbene	193	C14H11N	000256-96-2	50
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
4	2-Phenylindolizine	193	C14H11N	025379-20-8	50
5	3,4-Diethoxy-N-(4,5,6,7-tetrahyd...	346	C18H22N2O3S	1000311-37-1	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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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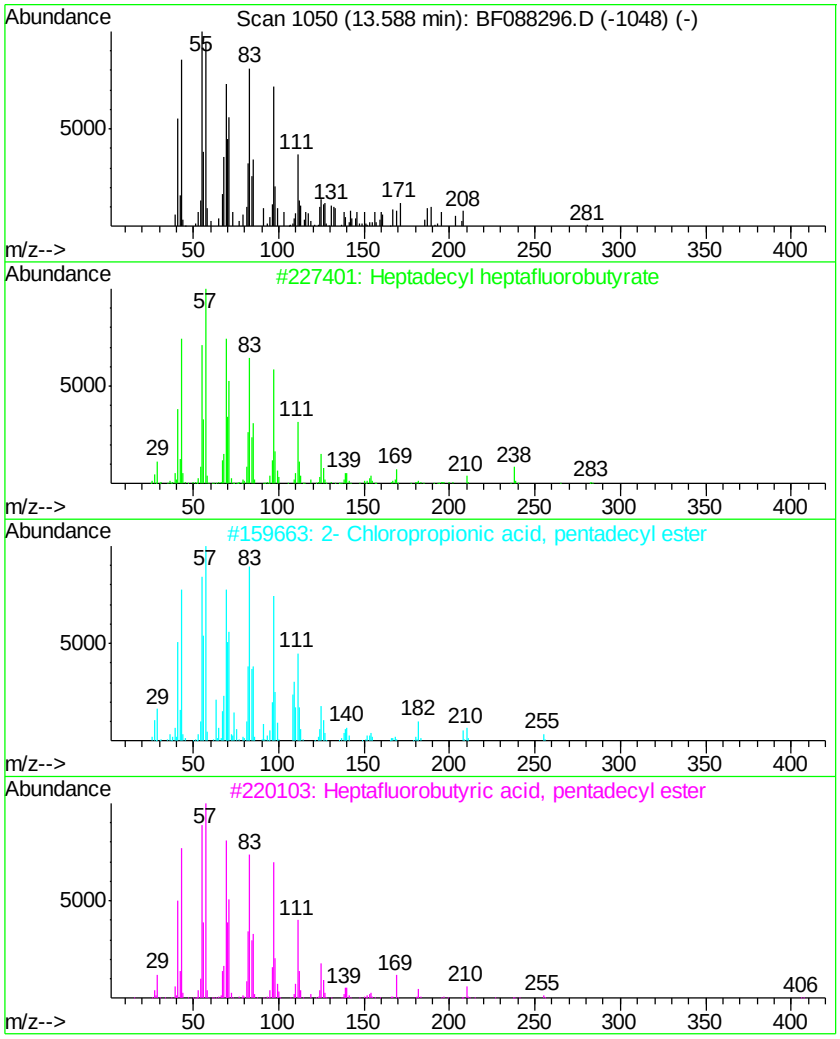
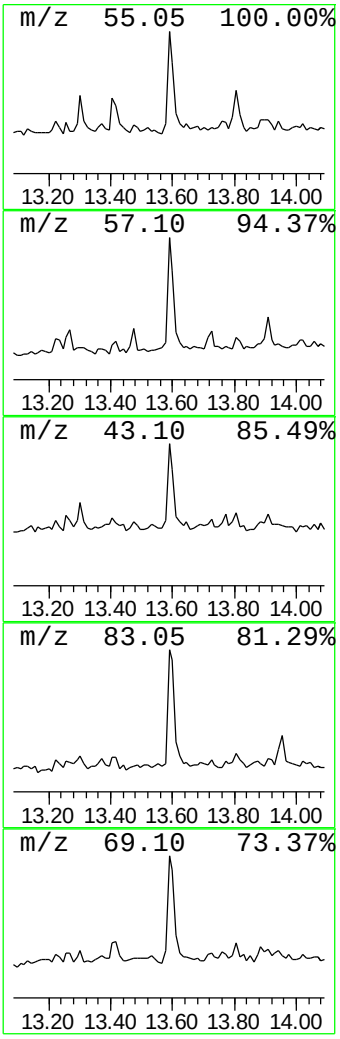
Peak Number 14 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	1.52 ng	108176	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088296.D
Acq On : 23 Jun 2016 18:17
Operator : UM/SJ
Sample : H3084-14
Misc :
ALS Vial : 3 Sample Multiplier: 0.25

Instrument : BNA_F
ClientSampleId : LF017MW001-160512

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Chloroiodomethane	2.38	1.8	ng	34830	1	6.60	96473	20.0
1,3-Oxathiolane	4.01	3.4	ng	65890	1	6.60	96473	20.0
Hexanoic acid, 2-...	7.31	1.0	ng	38459	2	7.88	192882	20.0
Diethyltoluamide	10.02	0.8	ng	64629	3	9.63	393450	20.0
Heptadecane	10.07	0.6	ng	47368	3	9.63	393450	20.0
4-Methyl-N-(2-oxo...	10.72	0.5	ng	39834	4	11.11	392918	20.0
n-Hexadecanoic acid	11.66	3.0	ng	235498	4	11.11	392918	20.0
Octadecanoic acid	12.43	1.6	ng	115060	5	13.74	356183	20.0
3,4-Dimethylbenza...	13.30	1.1	ng	77929	5	13.74	356183	20.0
3-Phenylindole	13.42	0.5	ng	38517	5	13.74	356183	20.0
Heptadecyl heptaf...	13.59	1.5	ng	108176	5	13.74	356183	20.0