LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084915.D
Acq On : 6 Feb 2016 16:49
Operator : SJ/IZ
Sample : H1338-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF020116.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	4.796	234	237	247	rVB	478068	597876	4.25%	1.028%
2	5.242	274	276	279	rBV	1842812	2301628	16.38%	3.958%
3	6.305	367	369	372	rBV	1353060	1446852	10.30%	2.488%
4	6.430	377	380	382	rBV	4488280	4325994	30.78%	7.438%
5	6.613	393	396	398	rBV	1372808	1887701	13.43%	3.246%
6	6.659	398	400	402	rVB	1281059	1062467	7.56%	1.827%
7	6.705	402	404	407	rBV	594449	559862	3.98%	0.963%
8	6.819	411	414	416	rVV	4302065	4166095	29.65%	7.164%
9	7.230	447	450	453	rVB	2872913	3145197	22.38%	5.408%
10	7.848	501	504	506	rBV	182741	218379	1.55%	0.375%
11	7.950	510	513	515	rBV	1110013	1342109	9.55%	2.308%
12	8.499	555	561	564	rBV2	740533	1146188	8.16%	1.971%
13	8.579	564	568	572	rVV	6397549	14053138	100.00%	24.164%
14	8.682	574	577	580	rBV	2485683	3077506	21.90%	5.292%
15	9.025	604	607	610	rBV	4094167	5569605	39.63%	9.577%
16	9.425	640	642	643	rVV	143201	143655	1.02%	0.247%
17	9.459	643	645	647	rVV	340683	500665	3.56%	0.861%
18	9.699	663	666	668	rBV	1285669	1405206	10.00%	2.416%
19	10.122	701	703	706	rBV2	159415	235525	1.68%	0.405%
20	10.488	732	735	737	rBV	2766389	3254980	23.16%	5.597%
21	11.174	792	795	797	rVB	1477717	1280489	9.11%	2.202%
22	11.768	845	847	854	rVB	165964	234893	1.67%	0.404%
23	12.762	931	934	936	rBV	4346708	3982533	28.34%	6.848%
24	12.808	936	938	946	rVB	190333	290468	2.07%	0.499%
25	13.745	1018	1020	1023	rVV	108579	183550	1.31%	0.316%
26	13.802	1023	1025	1027	rVB	1016015	908587	6.47%	1.562%
27	15.174	1142	1145	1147	rBV	726188	835891	5.95%	1.437%

Sum of corrected areas: 58157039

LSC Report - Integrated Chromatogram

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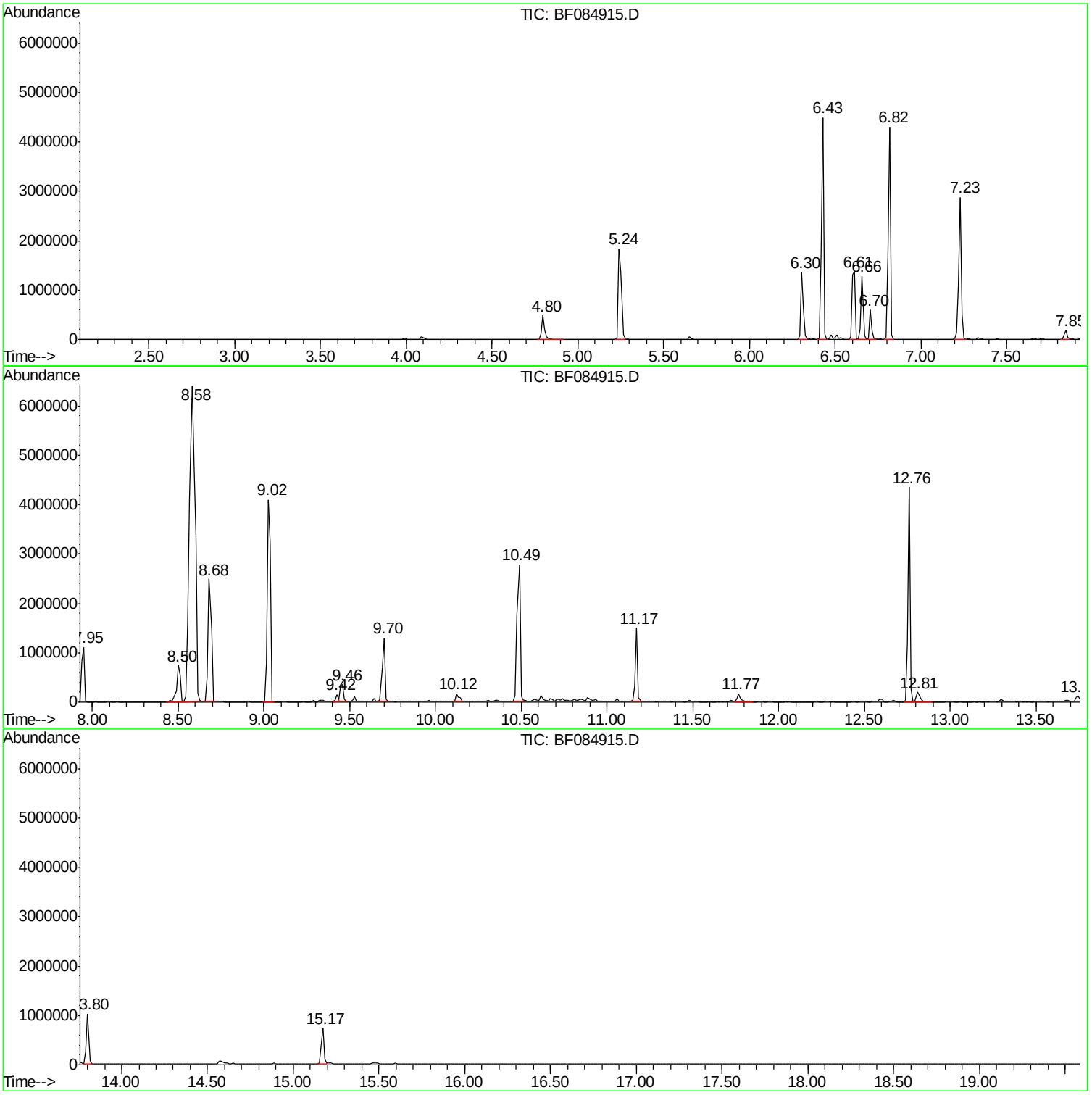
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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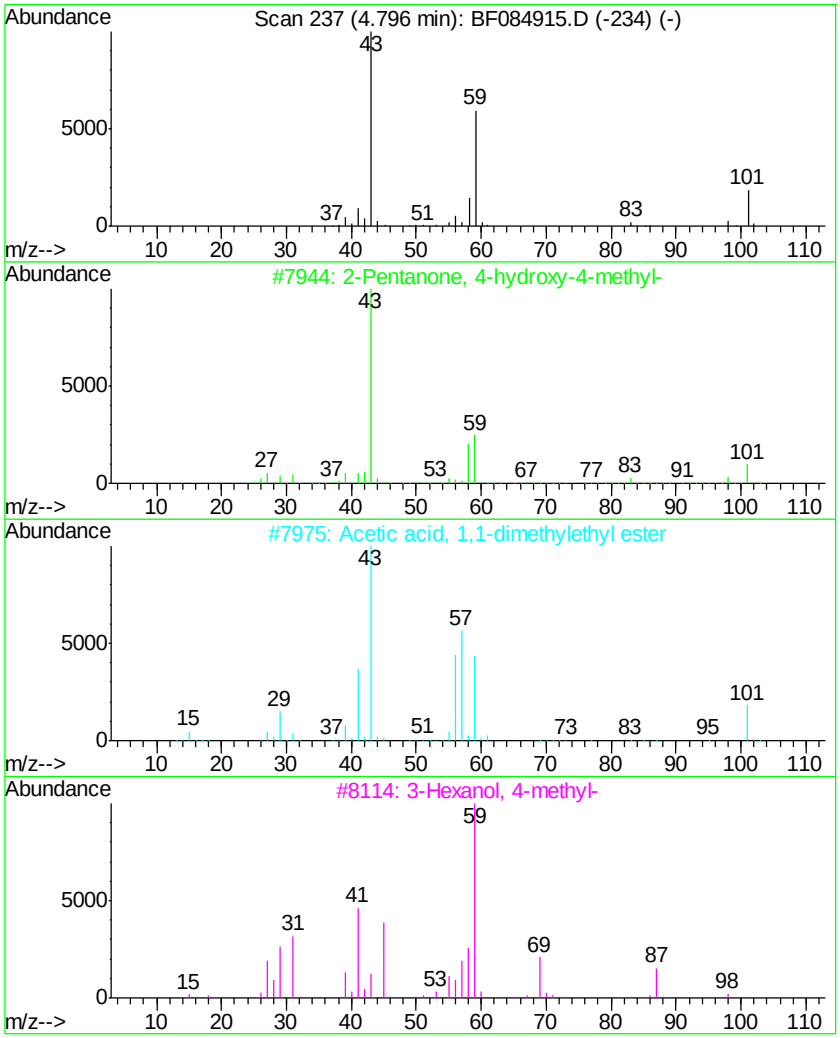
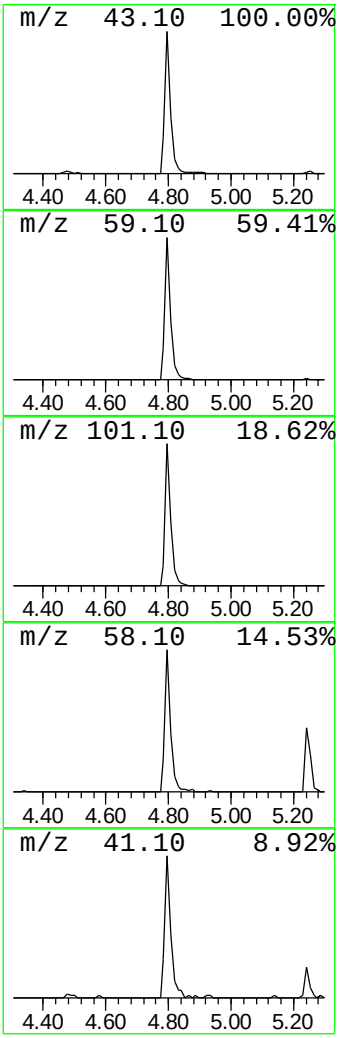
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	11.25 ng	597876	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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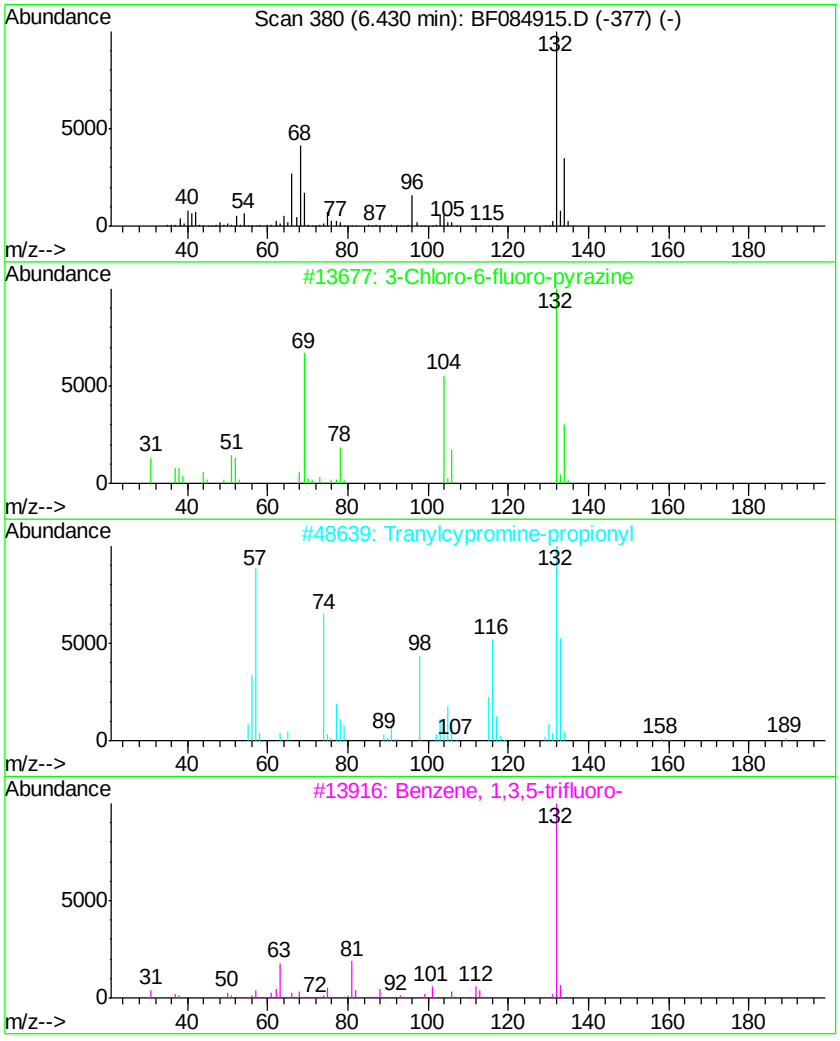
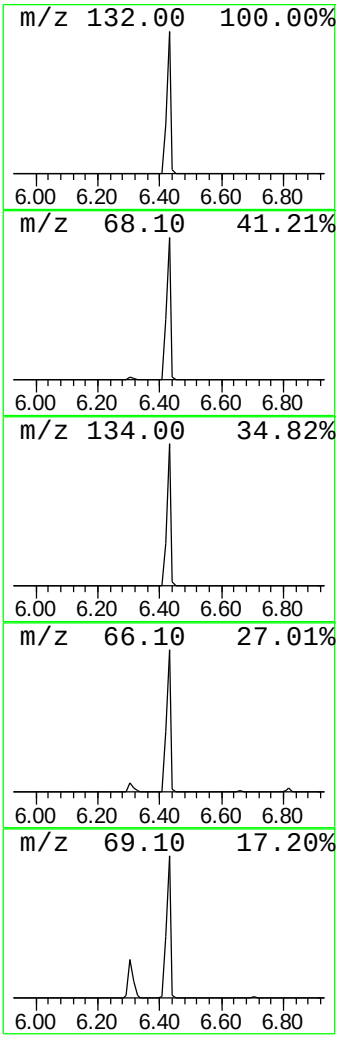
Peak Number 2 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	81.43 ng	4325990	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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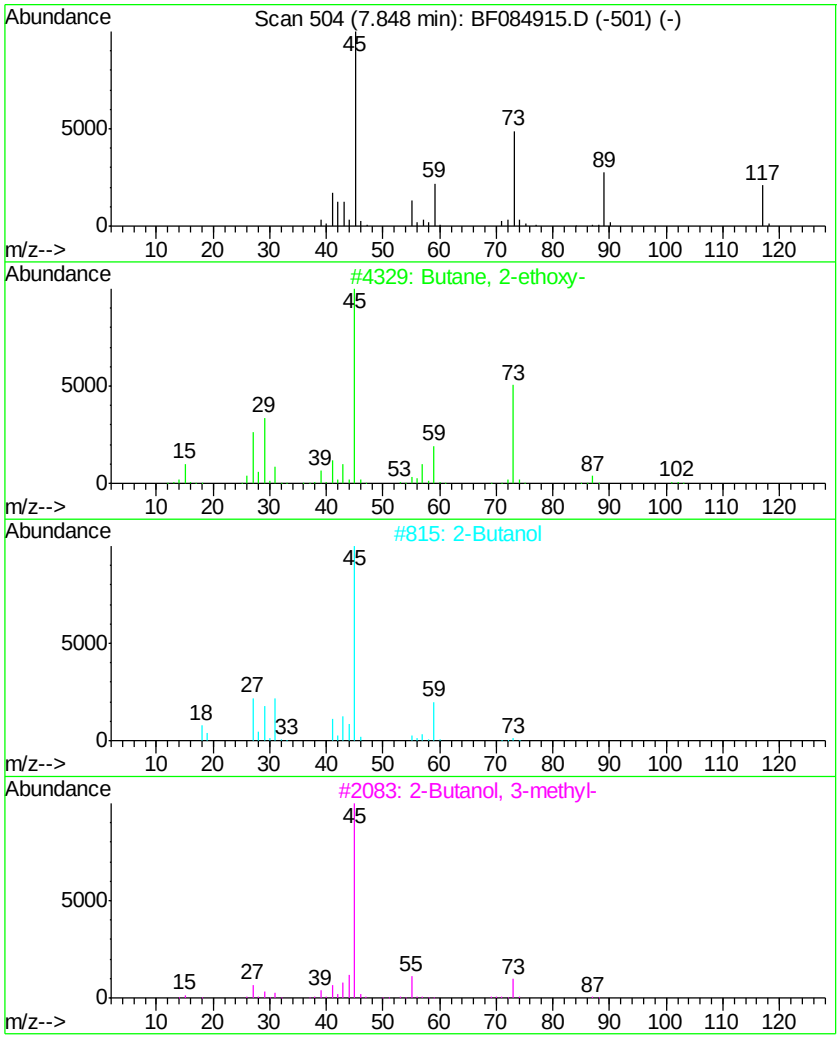
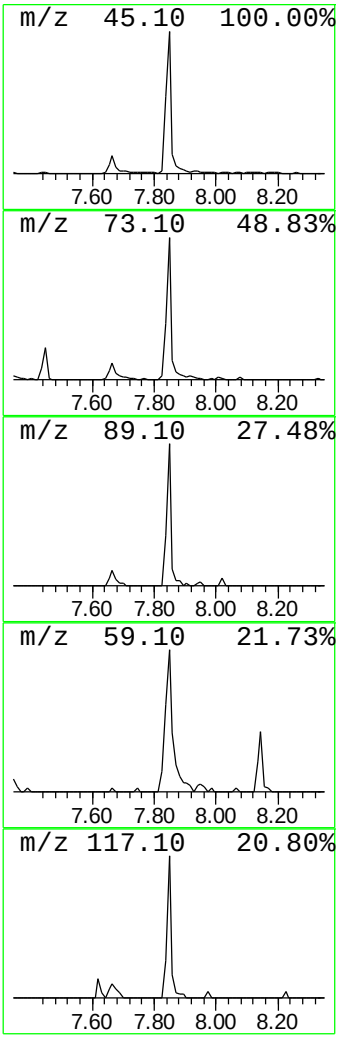
Peak Number 4 Butane, 2-ethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.85	3.25 ng	218379	Naphthalene-d8	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-ethoxy-	102	C6H14O	002679-87-0	50
2	2-Butanol	74	C4H10O	000078-92-2	38
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	38
4	Isoxazolidine	73	C3H7NO	000504-72-3	38
5	Propane, 1-(1-ethoxyethoxy)-	132	C7H16O2	020680-10-8	33





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ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
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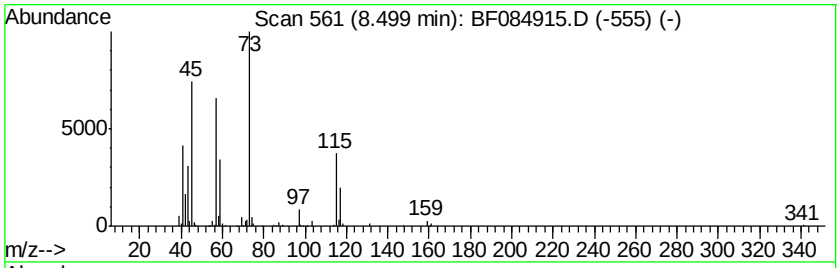
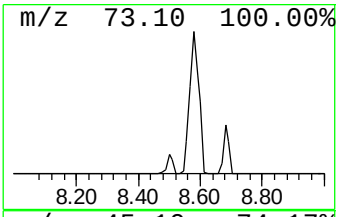
****

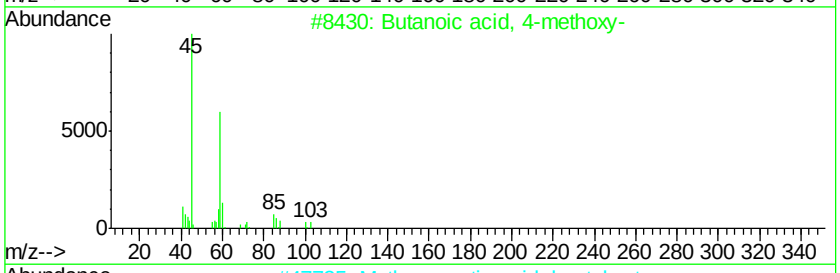
Peak Number 5 unknown8.50 Concentration Rank 5

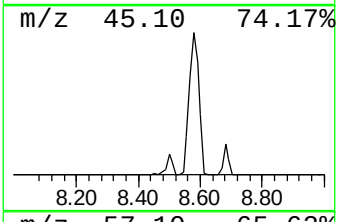
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	17.08 ng	1146190	Naphthalene-d8	7.95

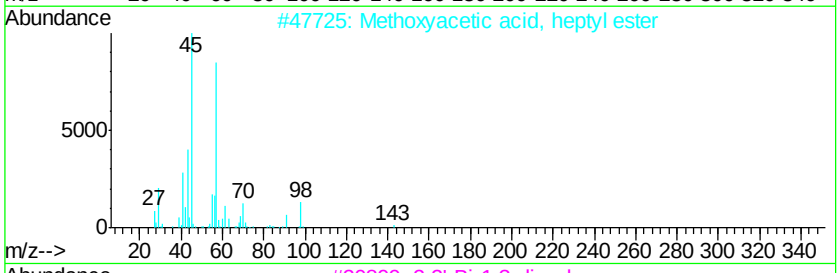
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	43
2	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	38
3	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	38
4	2H-Thiopyran-3(4H)-one	114	C5H6OS	029431-28-5	35
5	2-Pentenedioic acid, 2-methoxy-,...	188	C8H12O5	056009-33-7	33

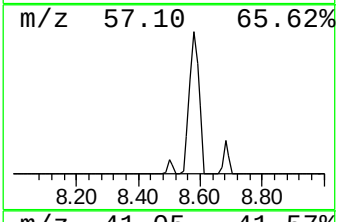


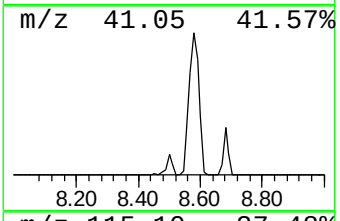


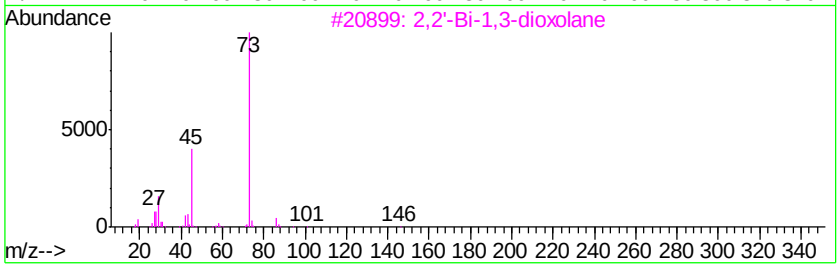


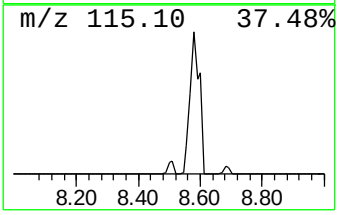












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Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

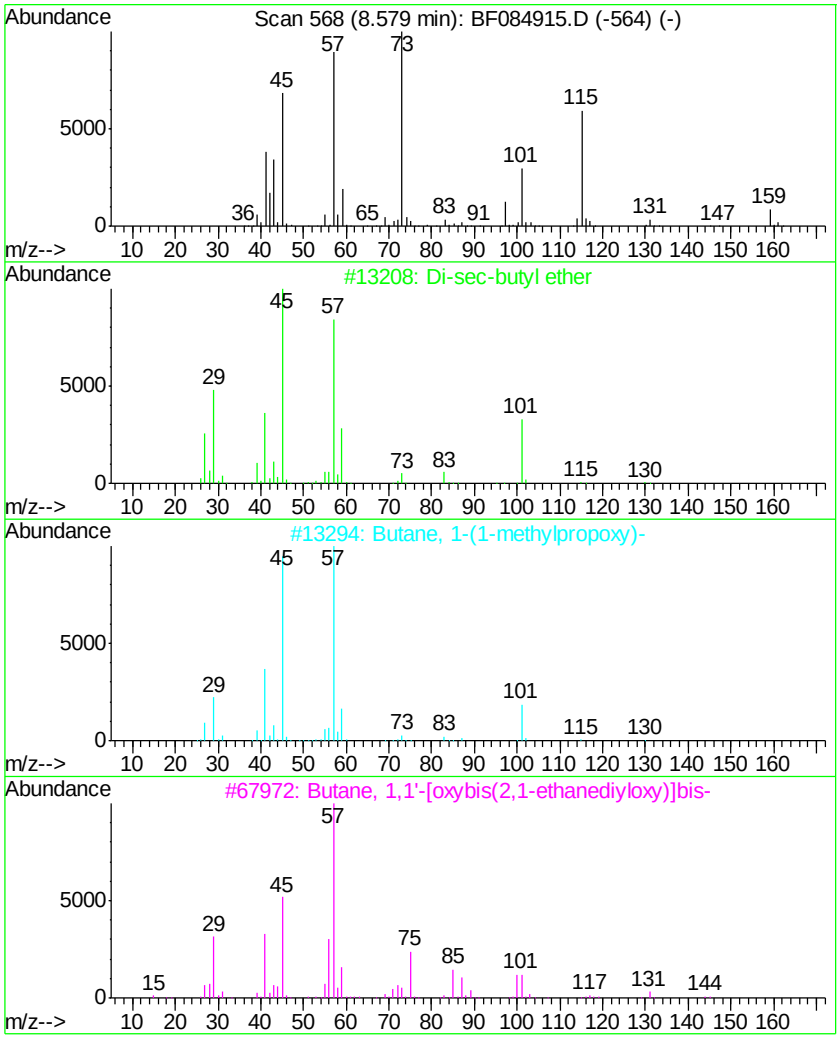
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

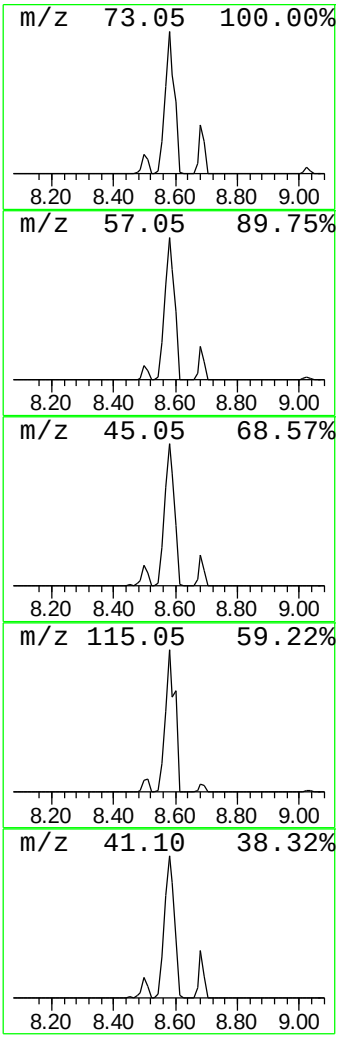
****

Peak Number 6 unknown8.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	209.42 ng	14053100	Naphthalene-d8	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-butyl ether	130	C8H18O	006863-58-7	35
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	32
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	32
4	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	27
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	25





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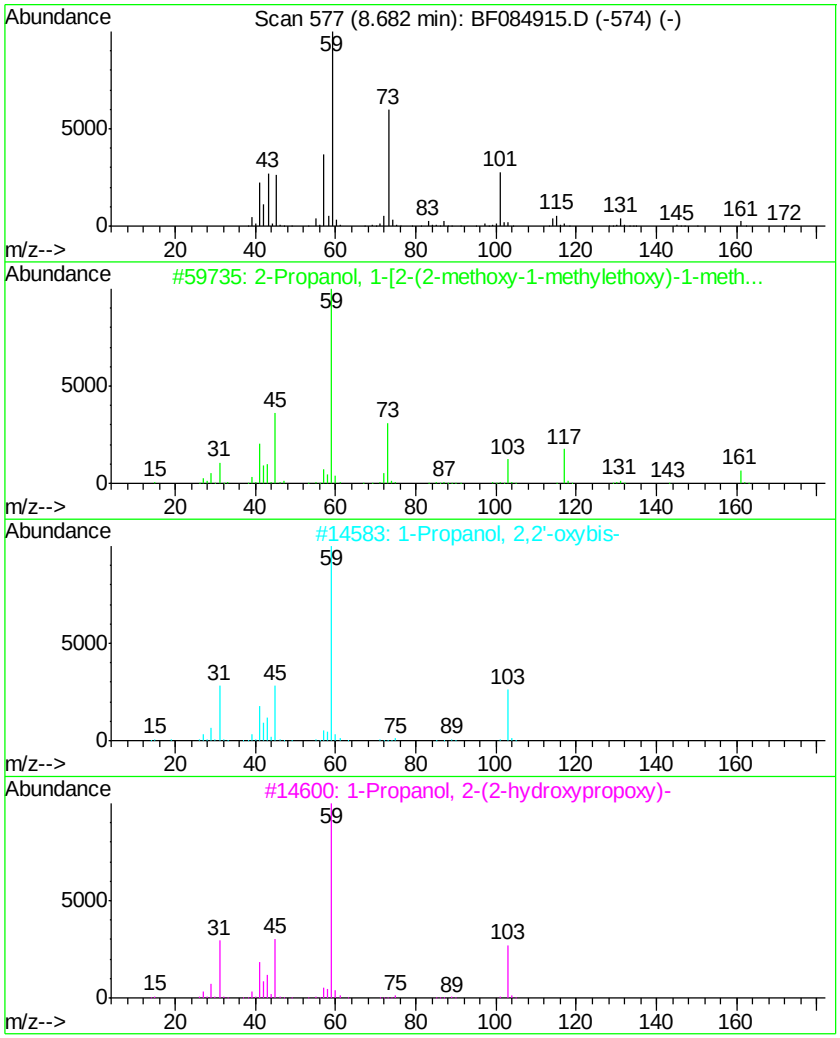
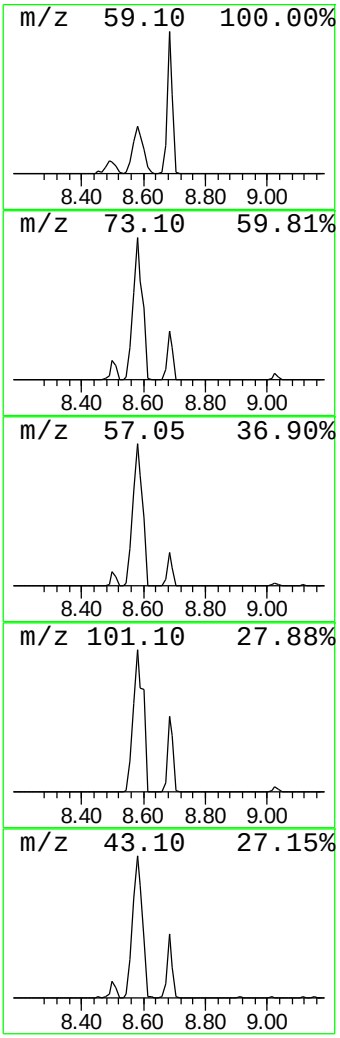
****

Peak Number 7 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	45.86 ng	3077510	Naphthalene-d8	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	50
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	45
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	45





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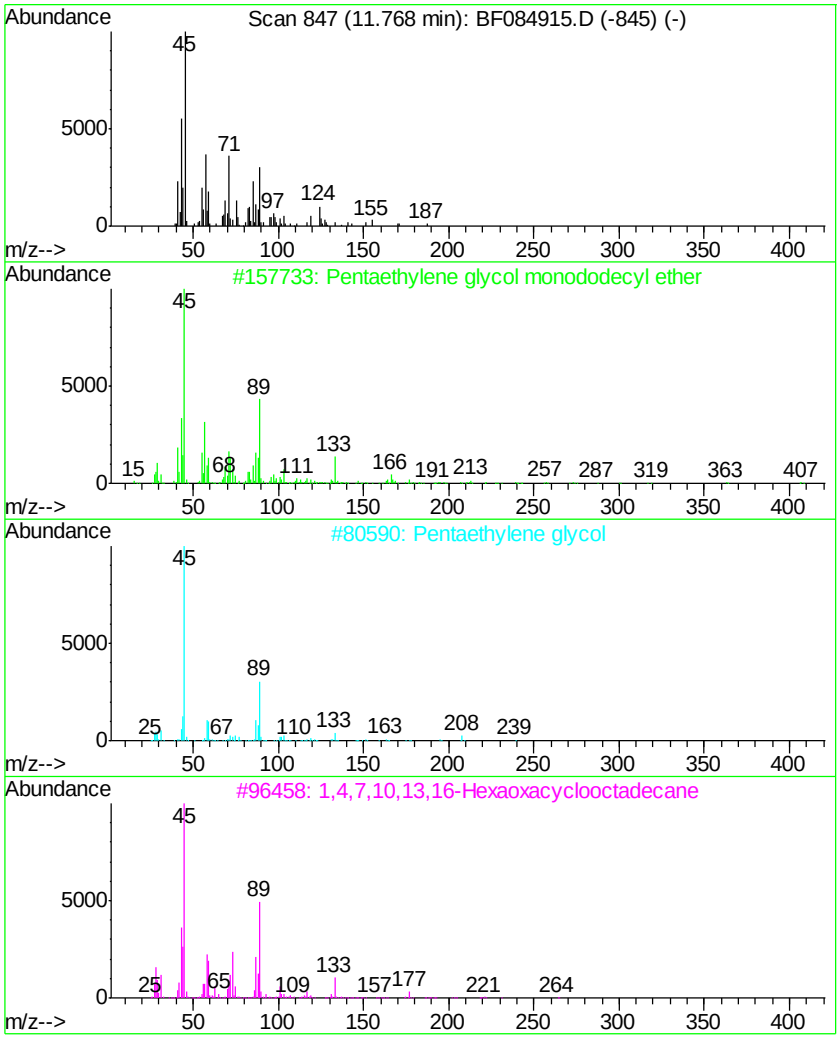
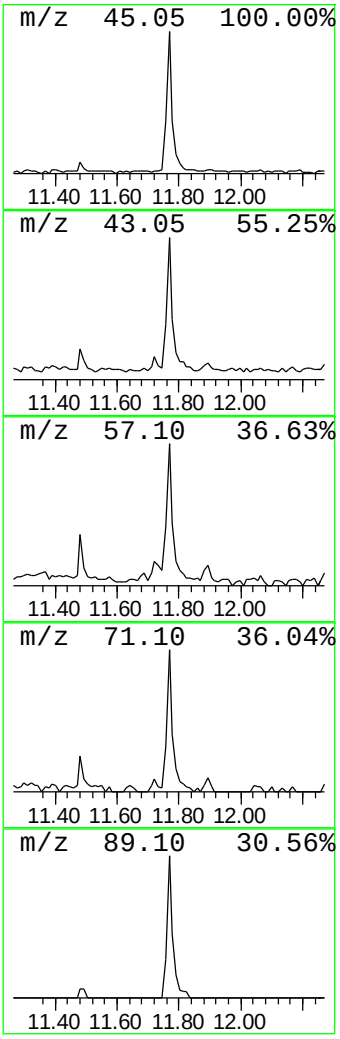
****

Peak Number 8 Pentaethylene glycol monodo... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.67 ng	234893	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	53
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
3	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	47
4	Hexagol	282	C12H26O7	002615-15-8	47
5	2-Octanol	130	C8H18O	000123-96-6	35





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

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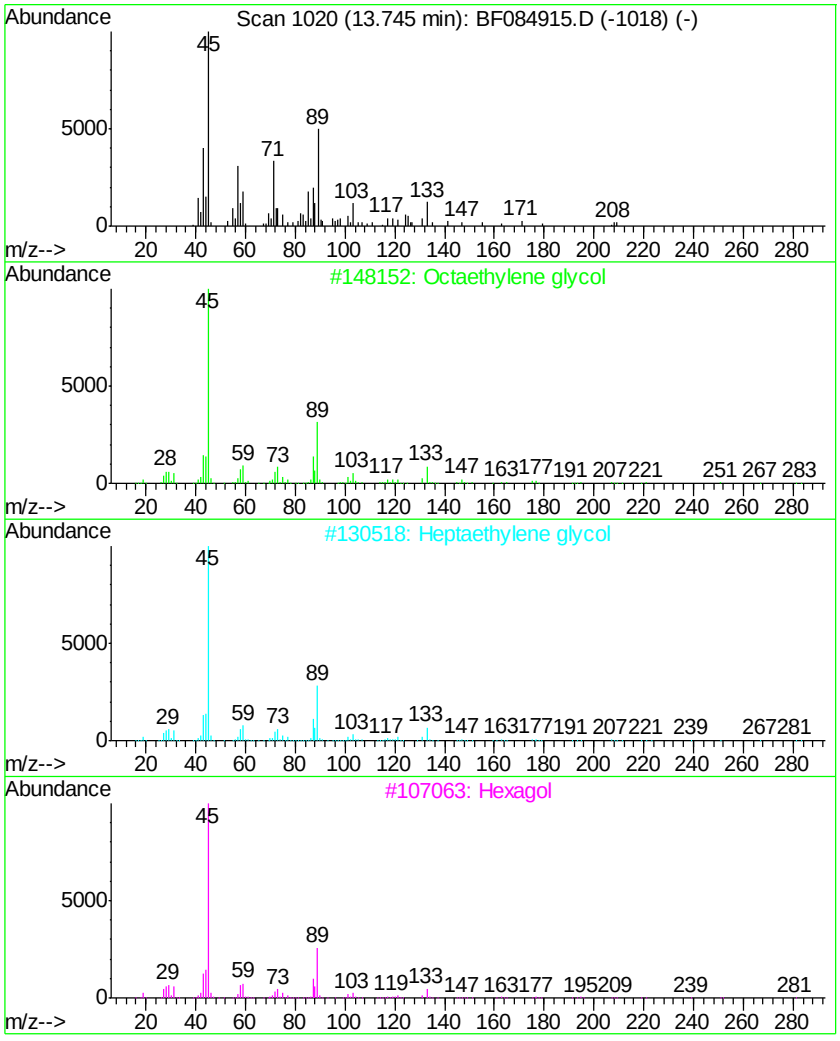
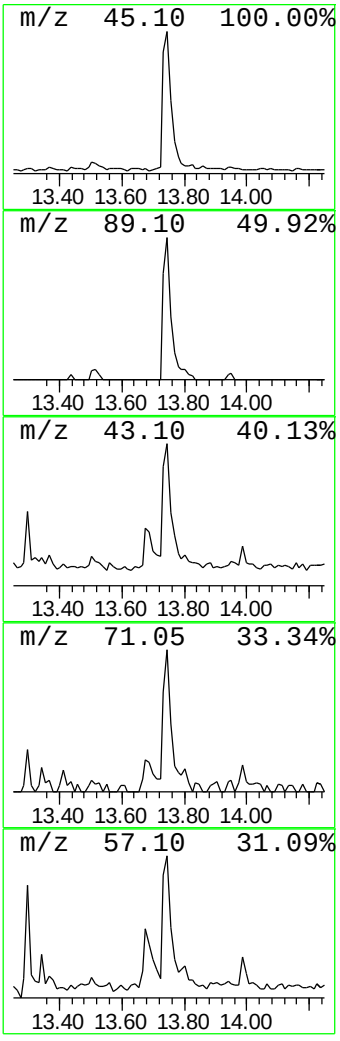
Peak Number 9 Octaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.04 ng	183550	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol	370	C16H34O9	1000289-34-2	83
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	80
3	Hexagol	282	C12H26O7	002615-15-8	64
4	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	64
5	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	59





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	11.3	ng	597876	1	6.66	1062470	20.0
unknown6.43	6.43	81.4	ng	4325990	1	6.66	1062470	20.0
Butane, 2-ethoxy-	7.85	3.3	ng	218379	2	7.95	1342110	20.0
unknown8.50	8.50	17.1	ng	1146190	2	7.95	1342110	20.0
unknown8.58	8.58	209.4	ng	14053100	2	7.95	1342110	20.0
2-Propanol, 1-[2-...	8.68	45.9	ng	3077510	2	7.95	1342110	20.0
Pentaethylene gly...	11.77	3.7	ng	234893	4	11.17	1280490	20.0
Octaethylene glycol	13.75	4.0	ng	183550	5	13.80	908587	20.0