

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094875.D
 Acq On : 4 May 2017 15:50
 Operator : SJ/MA
 Sample : I2940-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5040-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	2.266	53	56	61	rVB	34681	43361	1.96%	0.226%
2	4.107	364	369	377	rVB2	14389	27570	1.25%	0.144%
3	4.407	415	420	424	rBV	15812	24988	1.13%	0.130%
4	5.031	522	526	531	rBV	236910	411998	18.61%	2.146%
5	5.678	632	636	659	rBV	1003719	1557094	70.35%	8.112%
6	7.266	901	906	921	rBV	932714	1392998	62.94%	7.257%
7	7.384	921	926	935	rVB	1333239	1751787	79.15%	9.126%
8	7.725	979	984	994	rVB	394082	467642	21.13%	2.436%
9	7.960	1019	1024	1035	rBV	1185716	1363636	61.61%	7.104%
10	8.619	1130	1136	1146	rBV	835800	1066048	48.16%	5.554%
11	9.736	1322	1326	1338	rBV	509033	636458	28.76%	3.316%
12	11.513	1623	1628	1640	rBV	1847420	2109700	95.32%	10.990%
13	12.566	1802	1807	1816	rBV2	511359	693875	31.35%	3.615%
14	13.865	2022	2028	2037	rBV	865698	1148582	51.89%	5.984%
15	14.965	2211	2215	2228	rVB	558215	694118	31.36%	3.616%
16	15.942	2372	2381	2394	rBV	276402	384826	17.39%	2.005%
17	16.124	2407	2412	2418	rBV5	19612	25094	1.13%	0.131%
18	16.848	2529	2535	2538	rBV2	23493	27109	1.22%	0.141%
19	16.912	2543	2546	2553	rVB4	31091	47006	2.12%	0.245%
20	17.036	2560	2567	2579	rBV	445922	610600	27.59%	3.181%
21	17.301	2606	2612	2615	rBV	1858183	2213333	100.00%	11.530%
22	18.095	2744	2747	2756	rVB	19627	30258	1.37%	0.158%
23	18.442	2801	2806	2809	rBV	43426	67394	3.04%	0.351%
24	18.489	2810	2814	2817	rVV	72206	106265	4.80%	0.554%
25	18.524	2817	2820	2828	rVB	506776	513674	23.21%	2.676%
26	18.636	2835	2839	2847	rVB	666936	775184	35.02%	4.038%
27	19.330	2950	2957	2967	rVB	17718	47717	2.16%	0.249%
28	19.859	3038	3047	3051	rBV9	17864	50817	2.30%	0.265%
29	20.059	3075	3081	3084	rBV2	22435	33996	1.54%	0.177%
30	20.294	3117	3121	3130	rVB	581882	741077	33.48%	3.861%
31	20.400	3136	3139	3146	rVB6	20974	35771	1.62%	0.186%
32	20.694	3184	3189	3194	rBV7	12098	30715	1.39%	0.160%
33	21.212	3272	3277	3281	rVB6	15646	27387	1.24%	0.143%
34	21.506	3323	3327	3333	rVB8	19218	37727	1.70%	0.197%

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Misc :
ALS Vial : 3 Sample Multiplier: 1

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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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

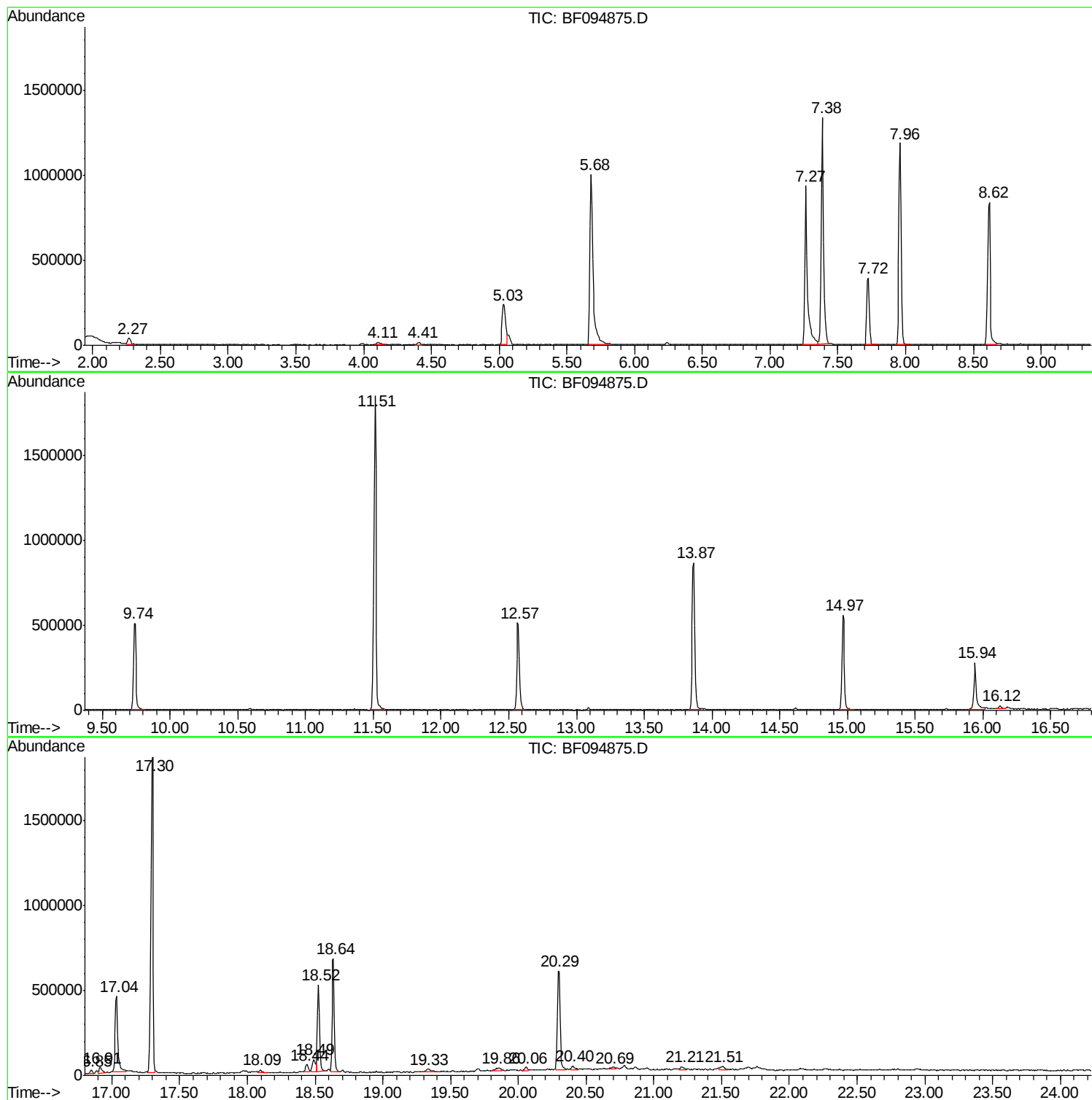
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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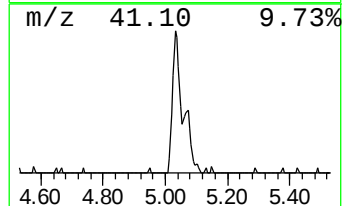
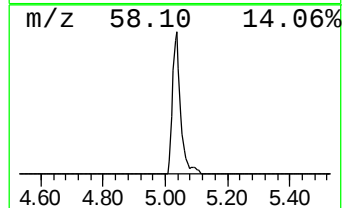
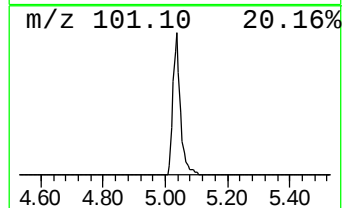
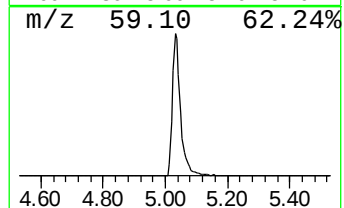
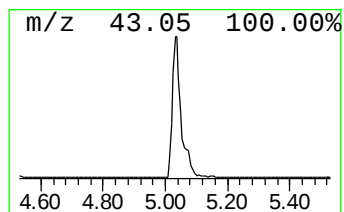
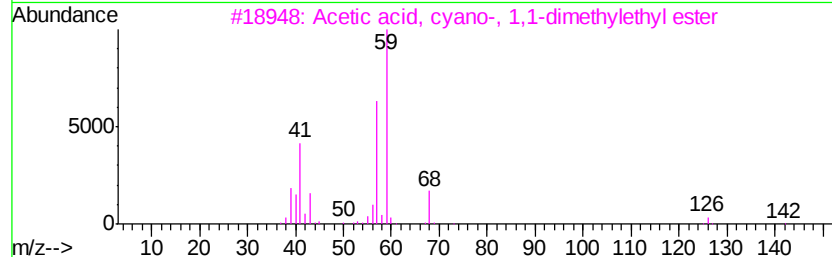
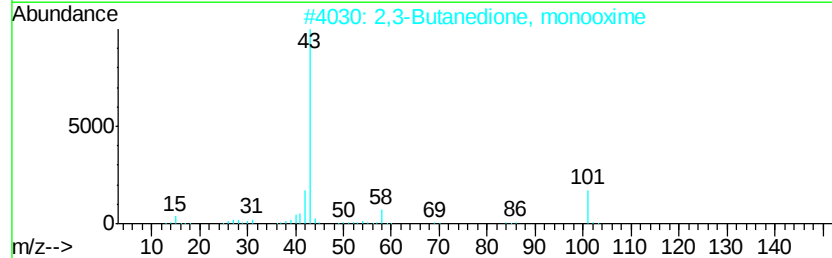
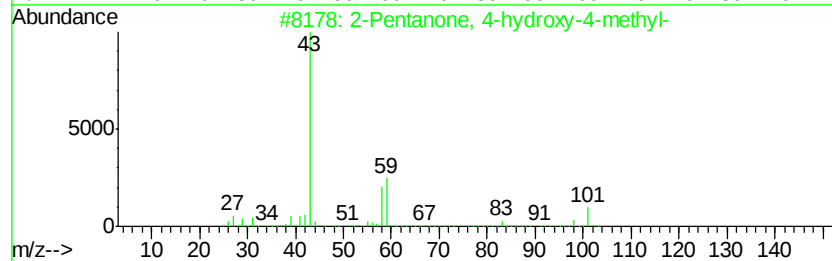
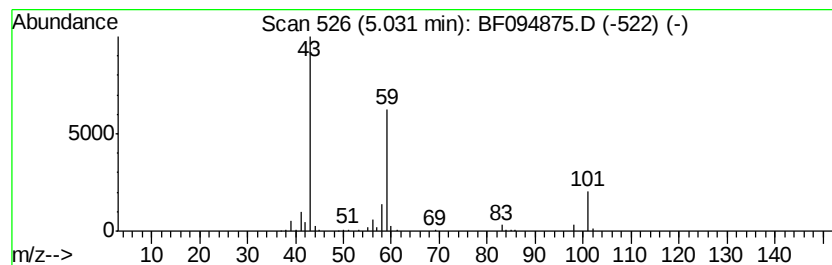
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	17.62 ng	411998	1,4-Dichlorobenzene-d4	7.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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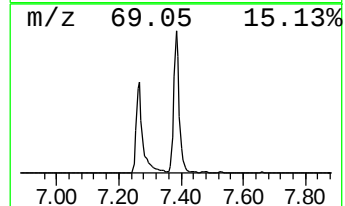
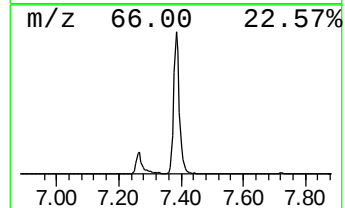
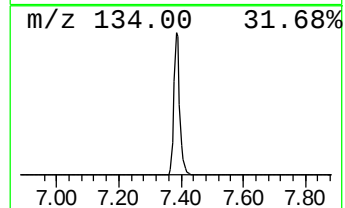
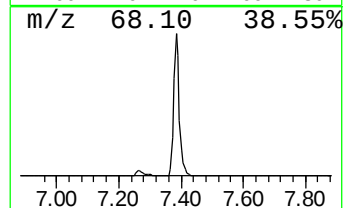
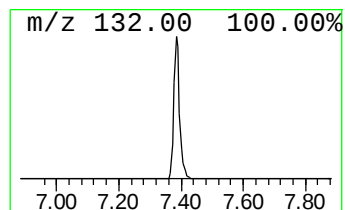
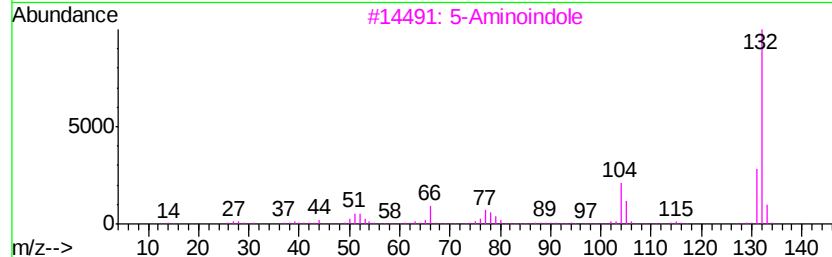
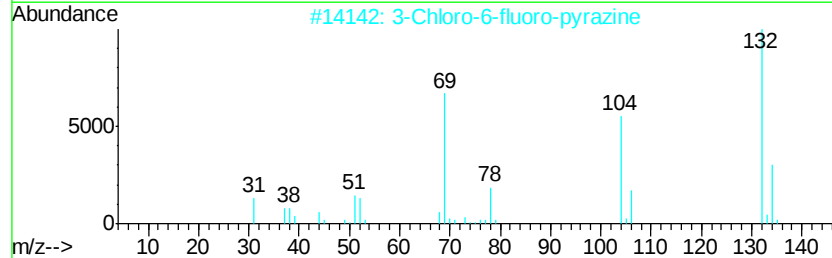
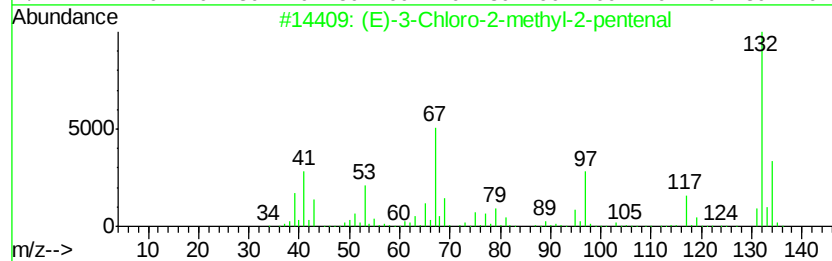
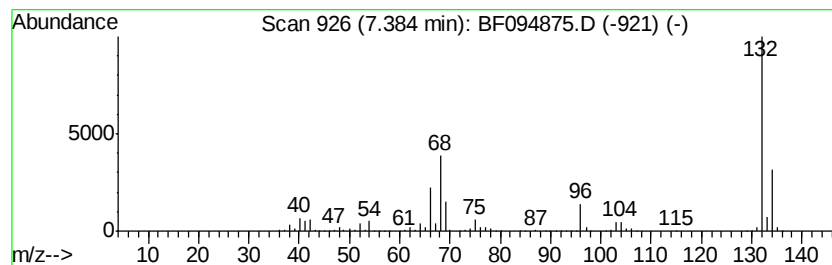
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (E)-3-Chloro-2-methyl-2-pen... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	74.92 ng	1751790	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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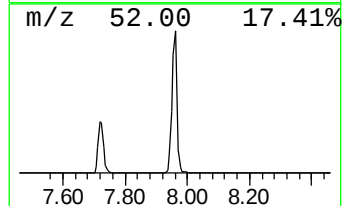
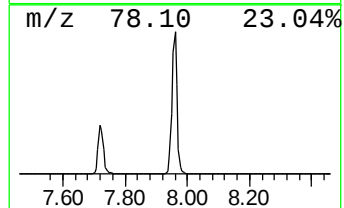
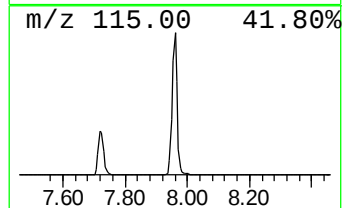
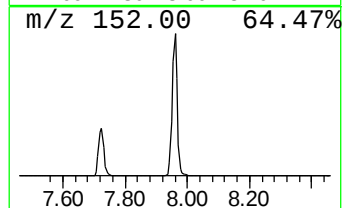
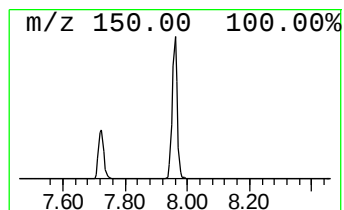
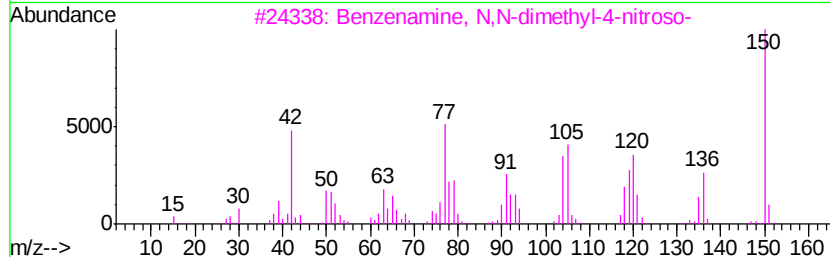
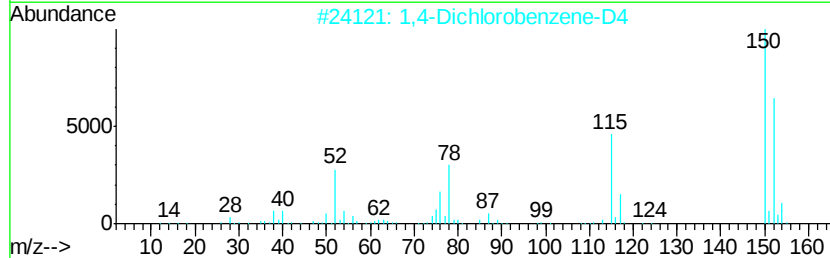
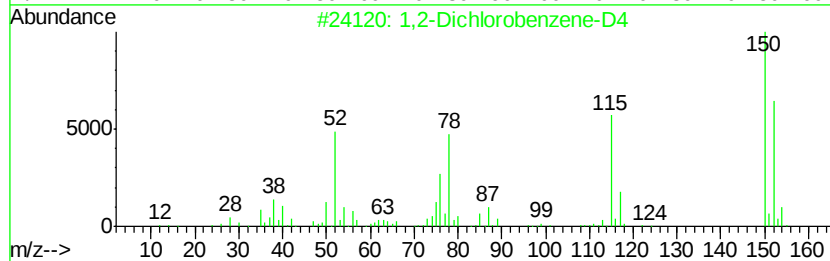
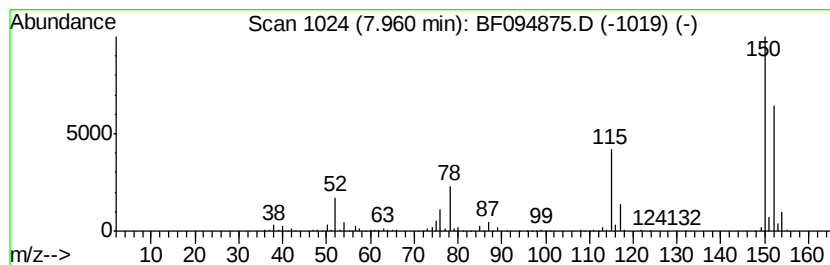
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	58.32 ng	1363640	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	95
2		1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
3		Benzenamine, N,N-dimethyl-4-nitr...	150	C8H10N2O	000138-89-6	32
4		9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	22
5		4,6-Diaminopyrazolo[3,4-d]pyrimi...	150	C5H6N6	005413-80-9	12



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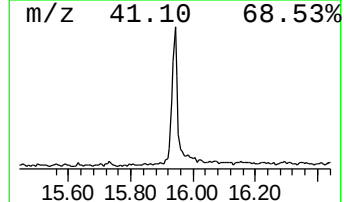
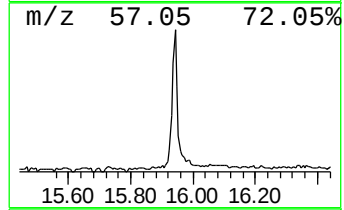
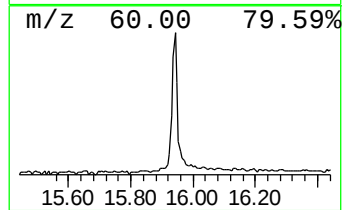
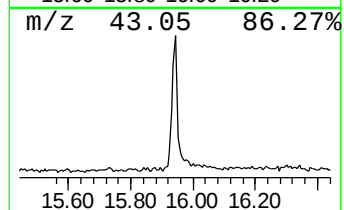
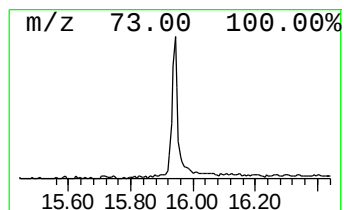
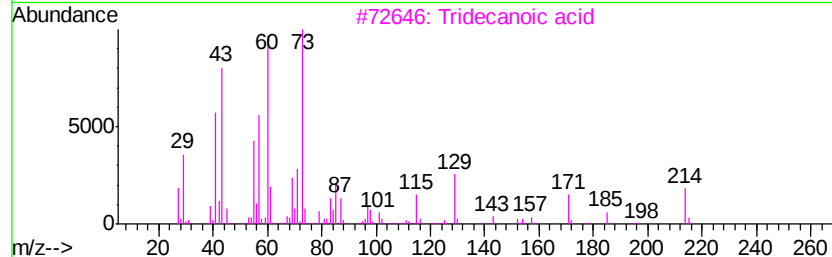
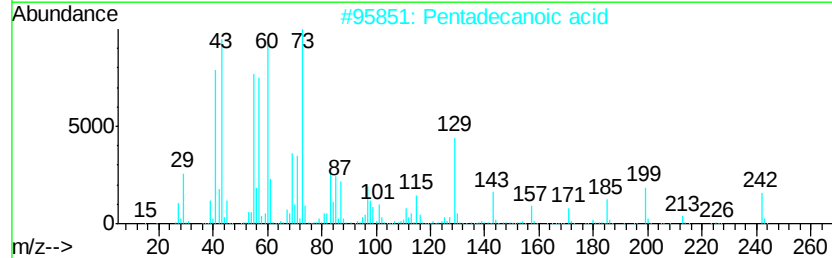
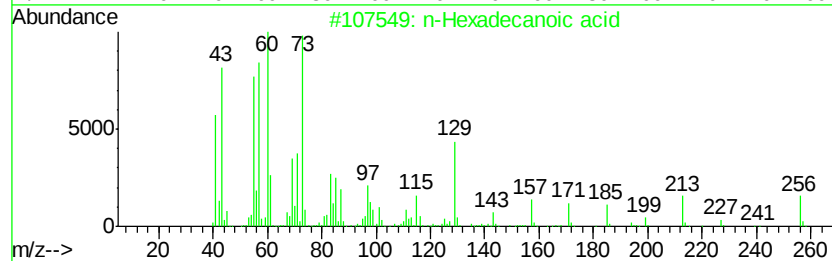
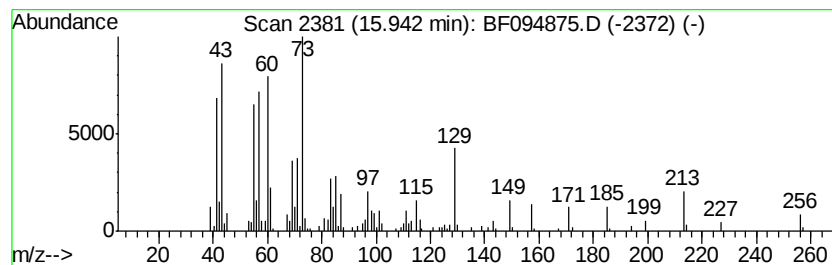
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	11.09 ng	384826	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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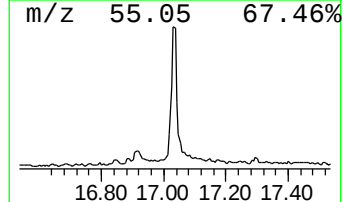
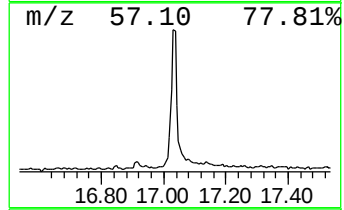
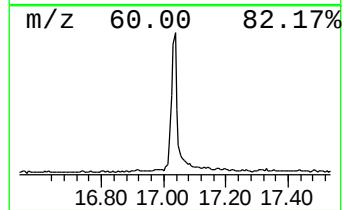
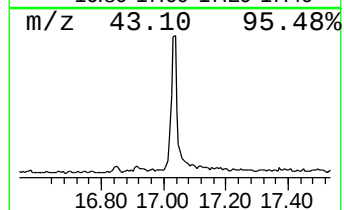
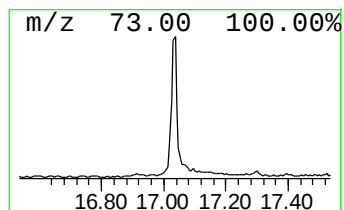
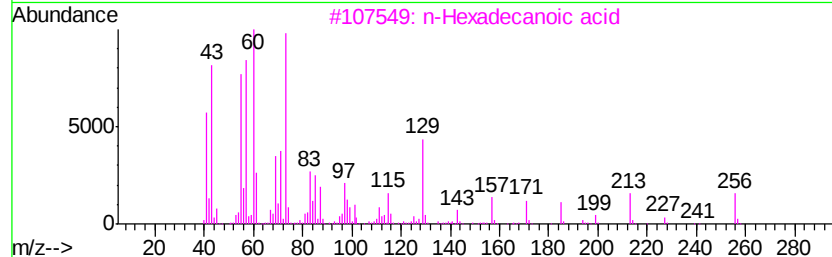
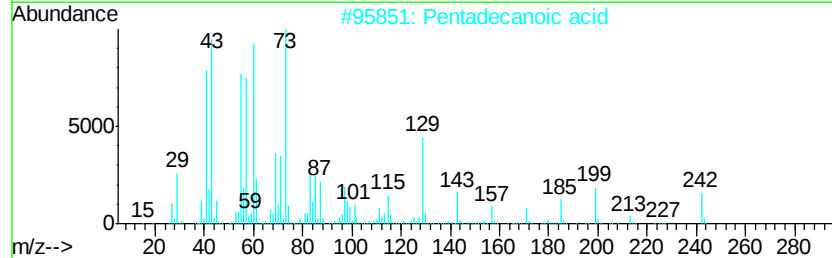
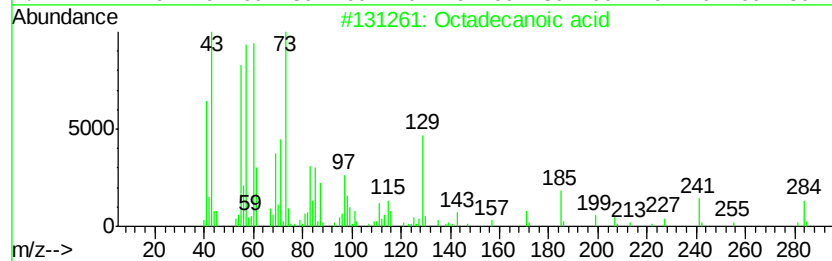
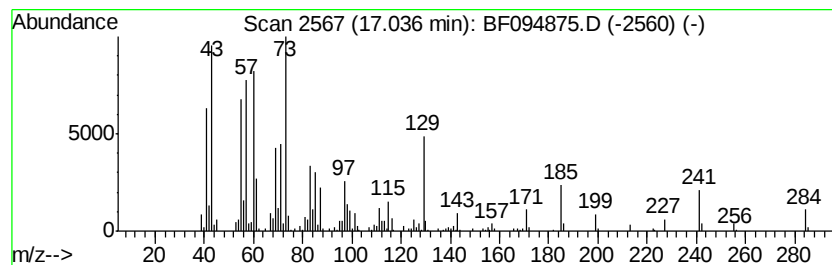
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	15.75 ng	610600	Chrysene-d12	18.64
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 89
3		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 87
4		Tetradecanoic acid	228 C14H28O2	000544-63-8 87
5		n-Decanoic acid	172 C10H20O2	000334-48-5 53



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Misc :
ALS Vial : 3 Sample Multiplier: 1

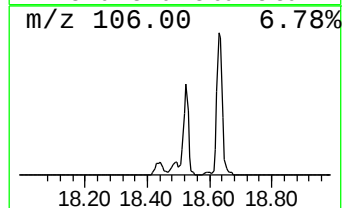
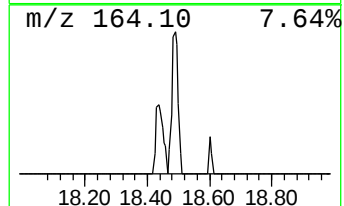
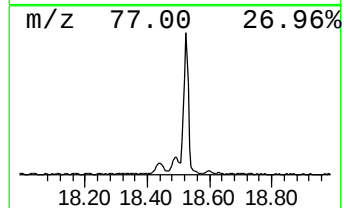
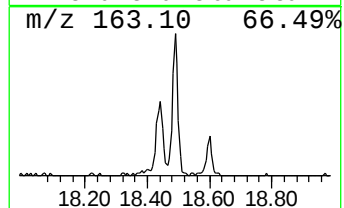
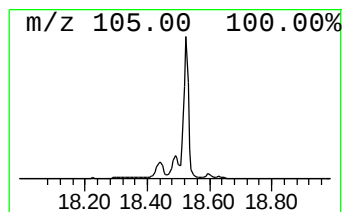
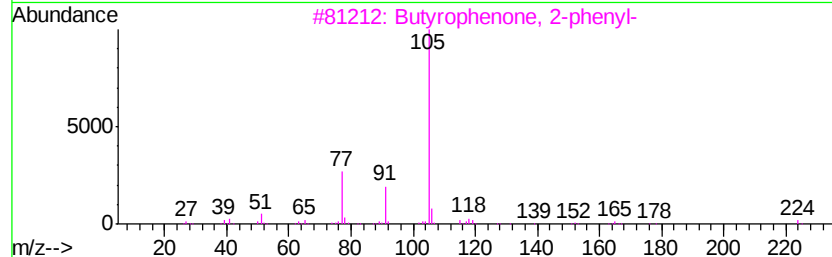
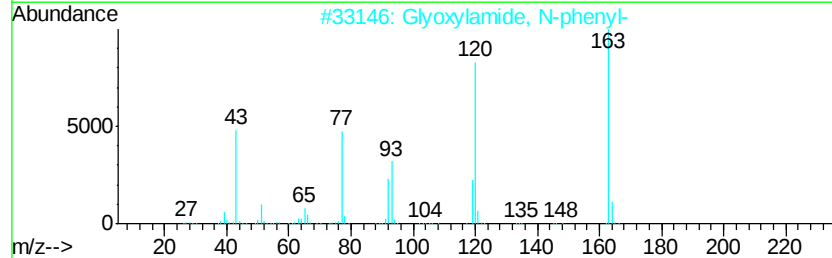
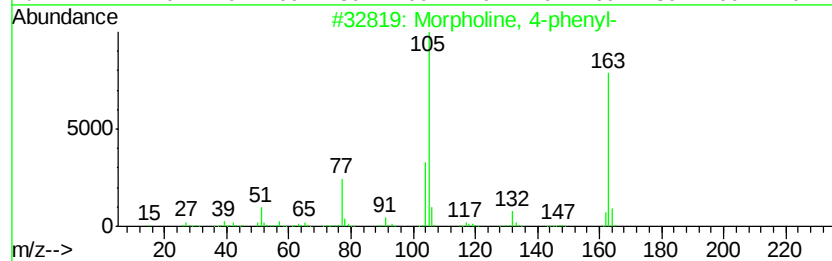
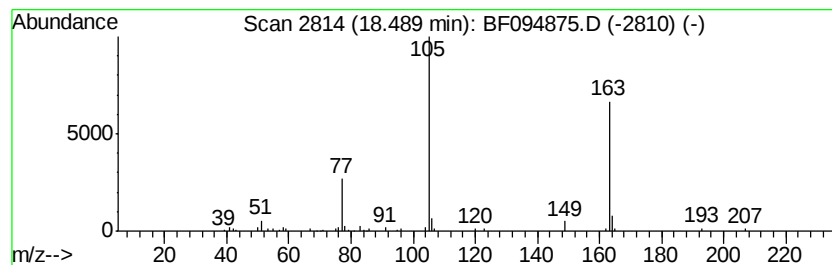
Instrument :
BNA_F
ClientSampleId :
5040-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Morpholine, 4-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.49	2.74 ng	106265	Chrysene-d12	18.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3	Butyrophenone, 2-phenyl-	224	C16H16O	016282-16-9	35
4	3,5-Dimethylphenyl isothiocyanate	163	C9H9NS	040046-30-8	33
5	Methyl nonyl phthalate	306	C18H26O4	091485-82-4	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094875.D
Acq On : 4 May 2017 15:50
Operator : SJ/MA
Sample : I2940-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

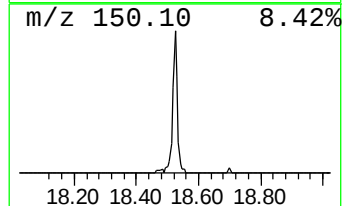
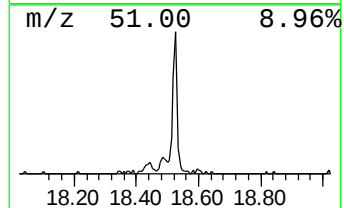
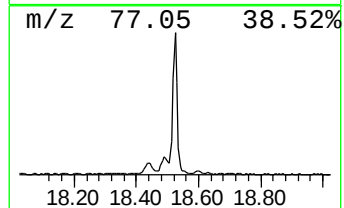
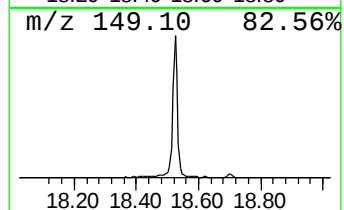
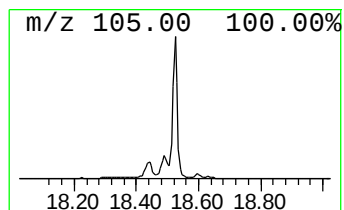
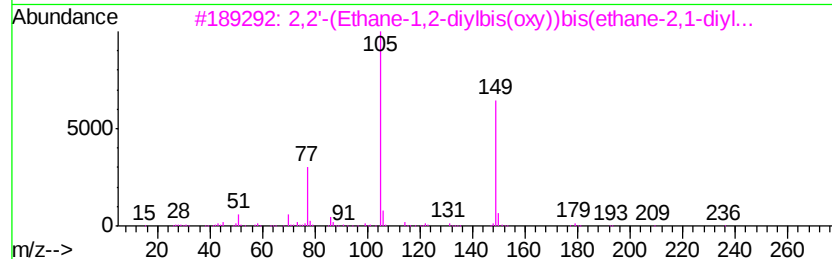
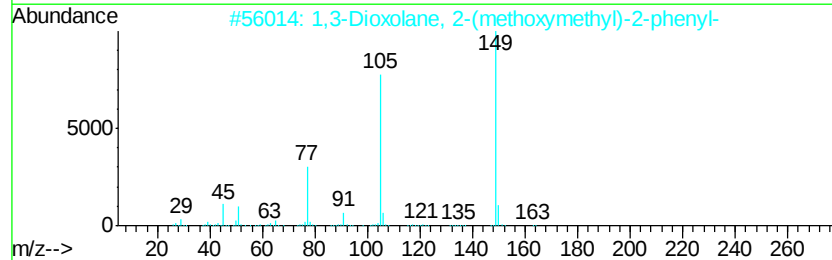
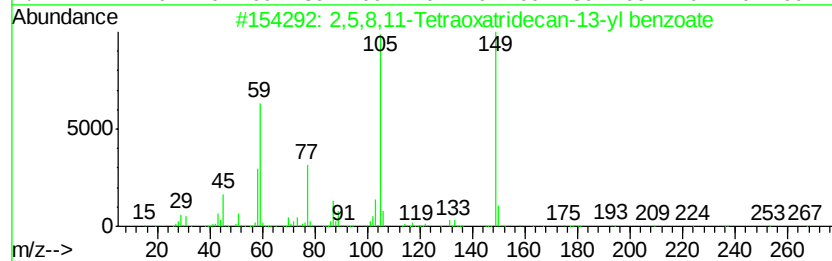
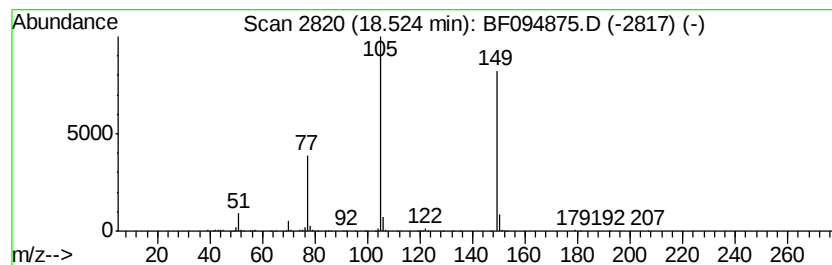
Instrument :
BNA_F
ClientSampleId :
5040-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,5,8,11-Tetraoxatridecan-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.52	13.25 ng	513674	Chrysene-d12	18.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	74
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094875.D
Acq On : 4 May 2017 15:50
Operator : SJ/MA
Sample : I2940-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5040-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	17.6	ng	411998	1	7.72	467642	20.0
(E)-3-Chloro-2-me...	7.38	74.9	ng	1751790	1	7.72	467642	20.0
1,2-Dichlorobenze...	7.96	58.3	ng	1363640	1	7.72	467642	20.0
n-Hexadecanoic acid	15.94	11.1	ng	384826	4	14.97	694118	20.0
Octadecanoic acid	17.04	15.8	ng	610600	5	18.64	775184	20.0
Morpholine, 4-phe...	18.49	2.7	ng	106265	5	18.64	775184	20.0
2,5,8,11-Tetraoxa...	18.52	13.3	ng	513674	5	18.64	775184	20.0