

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081716\
 Data File : BF089768.D
 Acq On : 17 Aug 2016 17:40
 Operator : UM/SJ
 Sample : H4476-04
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-19A

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-BF081616.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	6	7	16	rVB	1383601	2782987	7.84%	1.292%
2	1.793	16	18	75	rVB	12844755	35474726	100.00%	16.464%
3	4.833	282	284	287	rBV	1148928	1406134	3.96%	0.653%
4	5.279	320	323	325	rBV	5420396	7483477	21.10%	3.473%
5	6.330	412	415	417	rBV	4509022	4766902	13.44%	2.212%
6	6.467	424	427	429	rBV	10116048	13994575	39.45%	6.495%
7	6.696	445	447	449	rVB	4422210	3575903	10.08%	1.660%
8	6.856	458	461	463	rBV	13848498	12669633	35.71%	5.880%
9	7.267	493	497	499	rBV	10211318	11386753	32.10%	5.285%
10	7.668	526	532	536	rBV2	285462	866752	2.44%	0.402%
11	7.988	557	560	561	rBV	4257391	4728574	13.33%	2.195%
12	8.033	561	564	569	rVB4	179043	378120	1.07%	0.175%
13	9.073	651	655	657	rBV	15609642	20346820	57.36%	9.443%
14	9.462	685	689	691	rBV	397895	456946	1.29%	0.212%
15	9.736	710	713	715	rBV	6321953	5649904	15.93%	2.622%
16	9.942	728	731	735	rBV2	293509	451168	1.27%	0.209%
17	10.525	778	782	784	rBV	9174577	11582641	32.65%	5.376%
18	10.891	813	814	820	rVV2	247621	403343	1.14%	0.187%
19	11.211	839	842	844	rVV	6533353	5897869	16.63%	2.737%
20	11.268	844	847	851	rVB2	192245	364841	1.03%	0.169%
21	11.576	872	874	876	rBV	324026	402349	1.13%	0.187%
22	11.771	888	891	901	rBV2	4763031	7447793	20.99%	3.457%
23	12.399	944	946	949	rVB	555767	701260	1.98%	0.325%
24	12.559	957	960	964	rBV	6415650	7180765	20.24%	3.333%
25	12.628	964	966	971	rVB2	737648	1490405	4.20%	0.692%
26	12.708	971	973	976	rVB2	310317	509012	1.43%	0.236%
27	12.765	976	978	979	rBV	285938	472265	1.33%	0.219%
28	12.811	979	982	985	rVB	15331527	28621900	80.68%	13.284%
29	13.062	1001	1004	1006	rBV	608478	774822	2.18%	0.360%
30	13.291	1021	1024	1028	rBV	973630	1199325	3.38%	0.557%
31	13.371	1028	1031	1033	rBV	2065684	2809733	7.92%	1.304%
32	13.417	1033	1035	1036	rVB	1170008	1264764	3.57%	0.587%
33	13.691	1056	1059	1060	rBV	628250	867395	2.45%	0.403%
34	13.725	1060	1062	1063	rBV	923522	934422	2.63%	0.434%

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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

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35	13.760	1063	1065	1067	rVB	2646413	2472103	6.97%	1.147%
36	13.874	1072	1075	1079	rBV2	5749554	7864681	22.17%	3.650%
37	14.091	1092	1094	1097	rVB	567489	683745	1.93%	0.317%
38	14.434	1122	1124	1132	rVB	369140	555540	1.57%	0.258%
39	15.348	1201	1204	1207	rBV	3980527	4541997	12.80%	2.108%

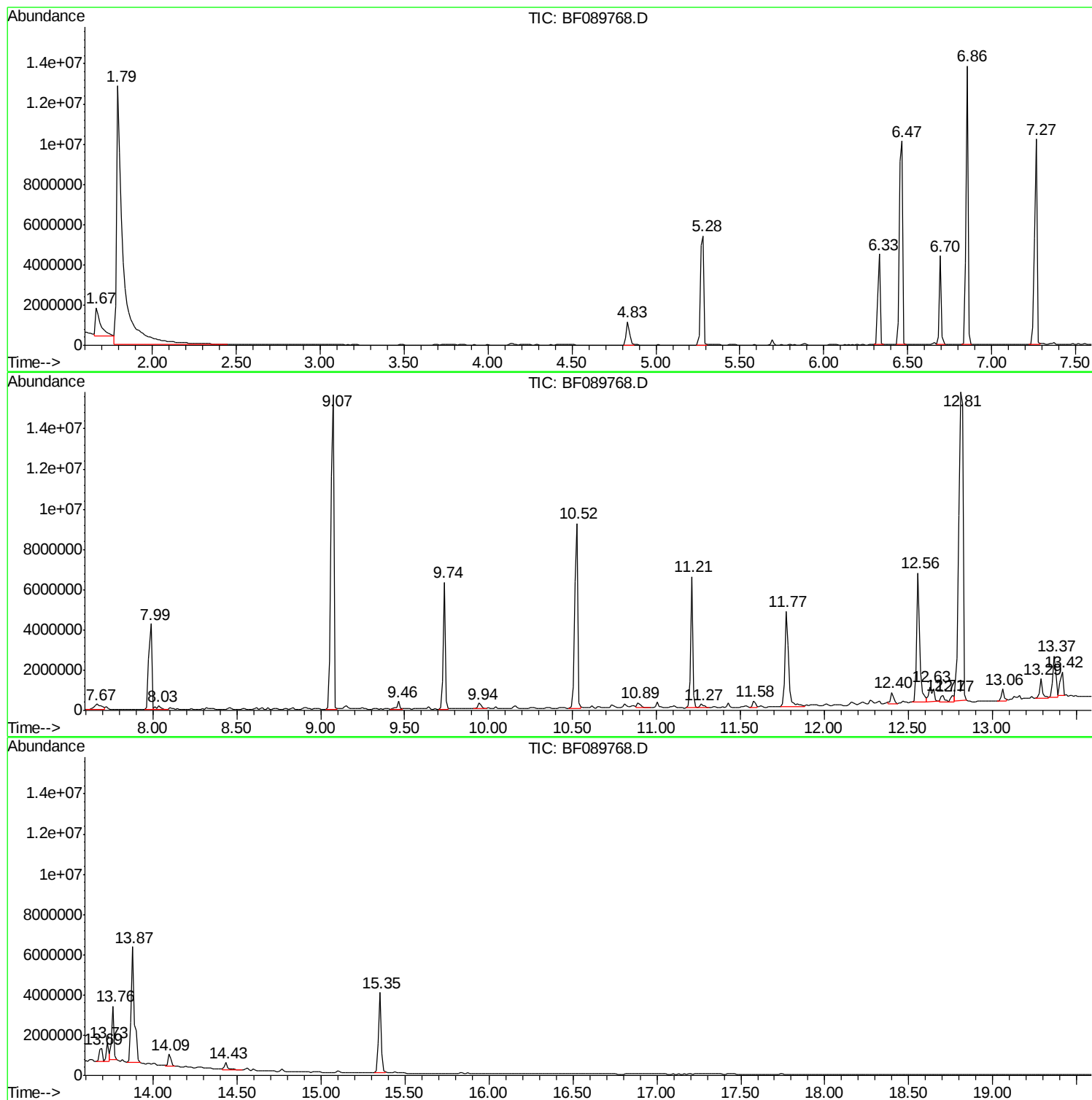
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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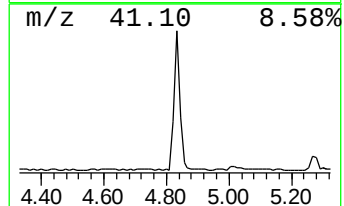
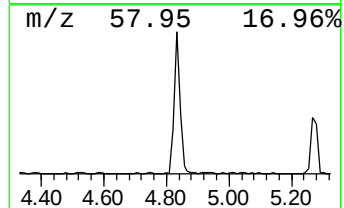
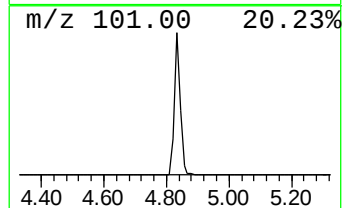
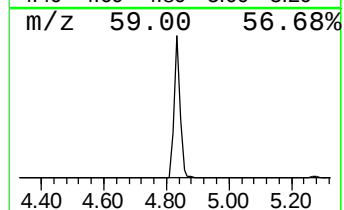
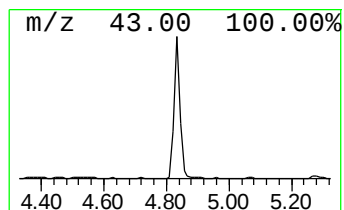
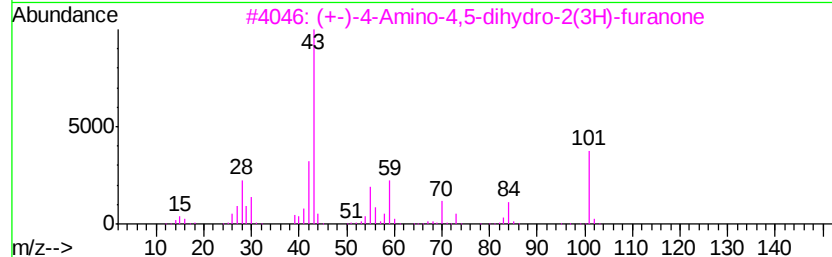
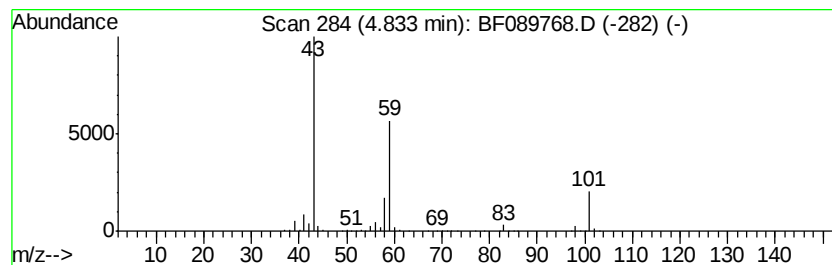
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	7.86 ng	1406130	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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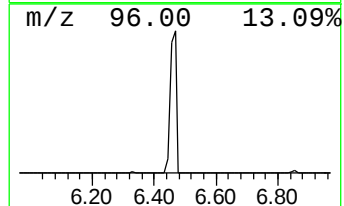
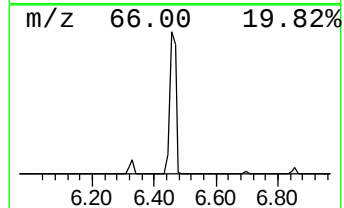
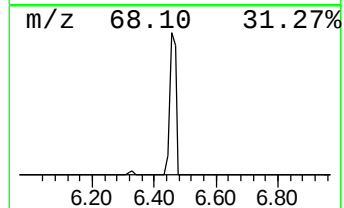
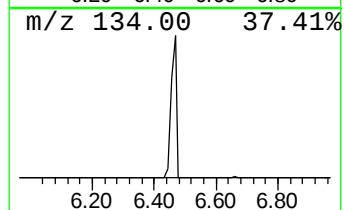
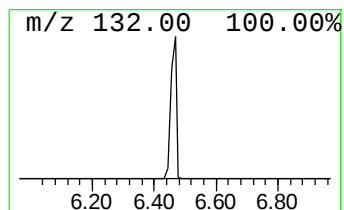
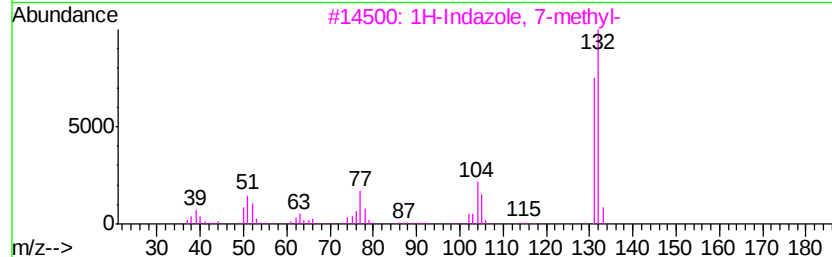
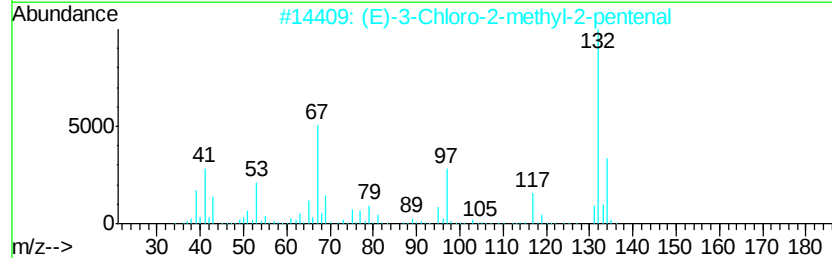
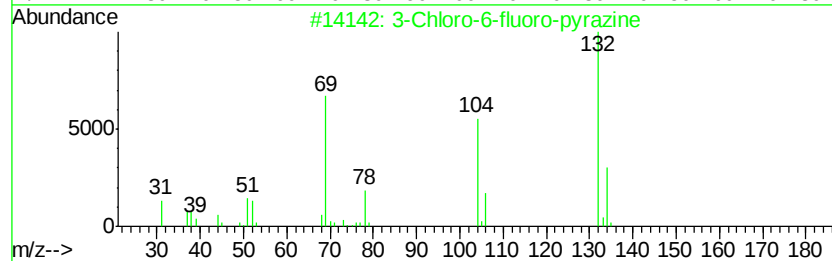
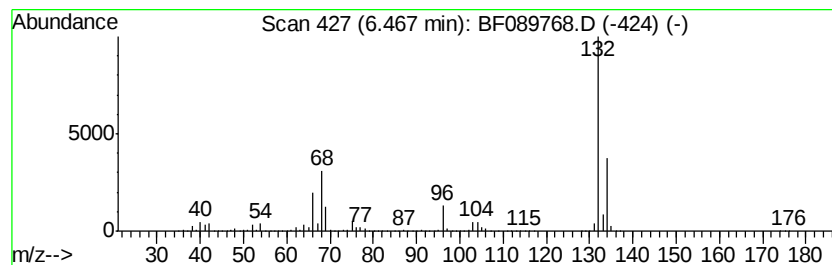
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.27 ng	13994600	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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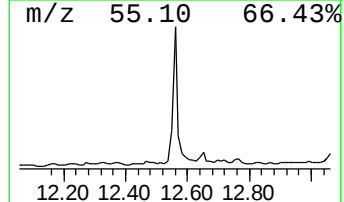
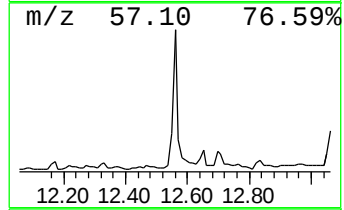
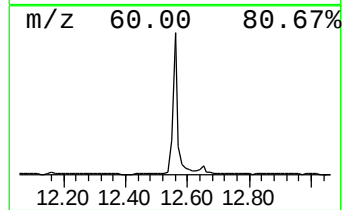
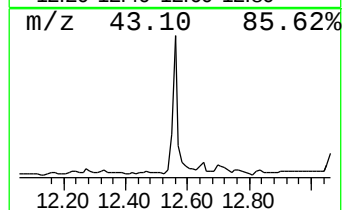
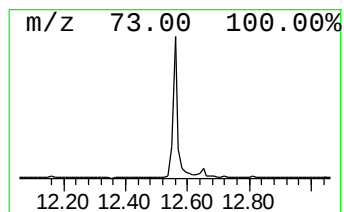
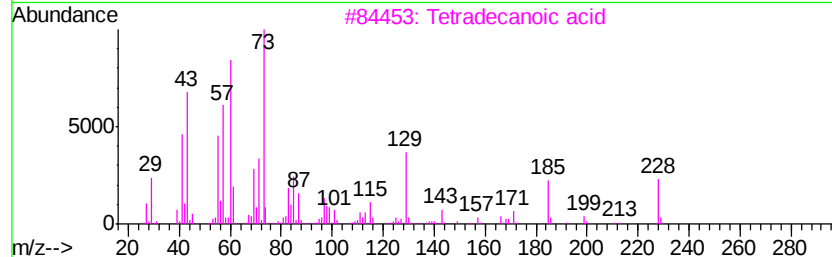
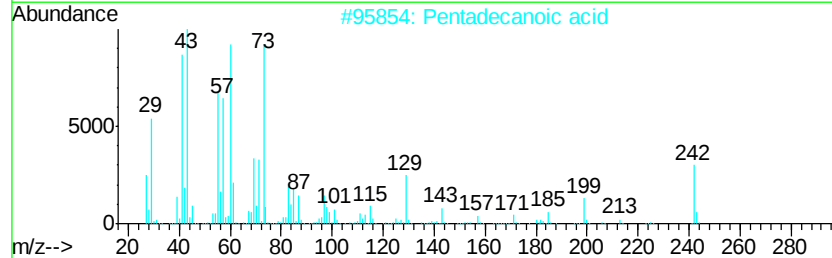
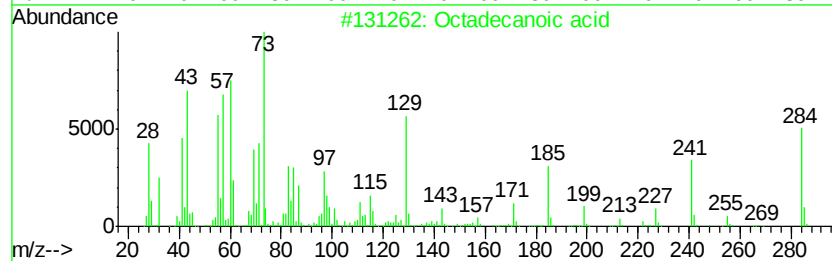
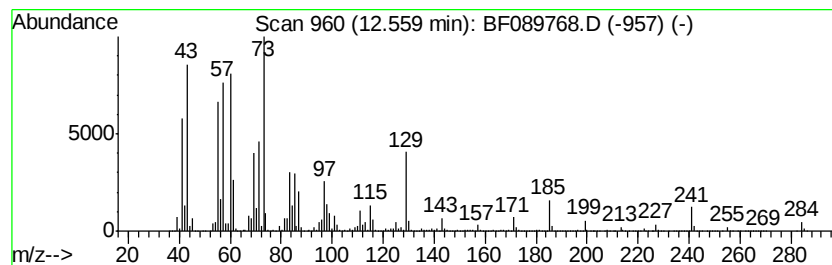
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	18.26 ng	7180770	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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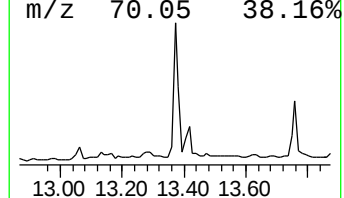
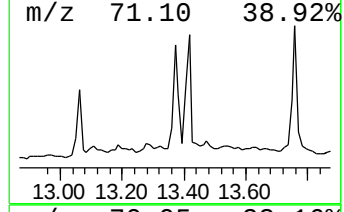
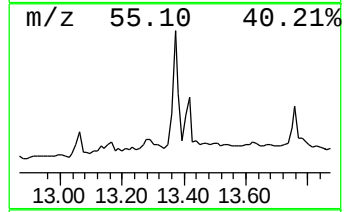
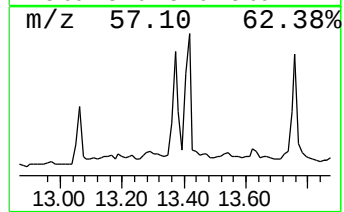
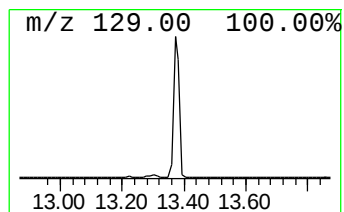
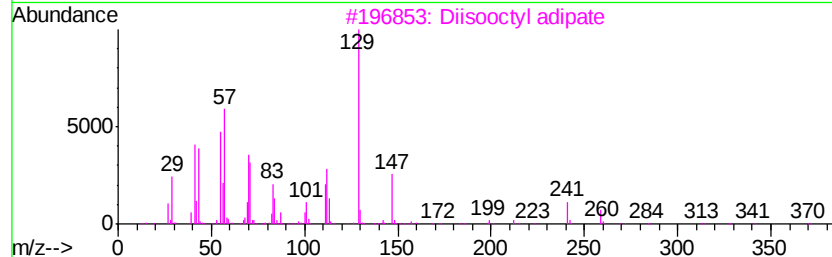
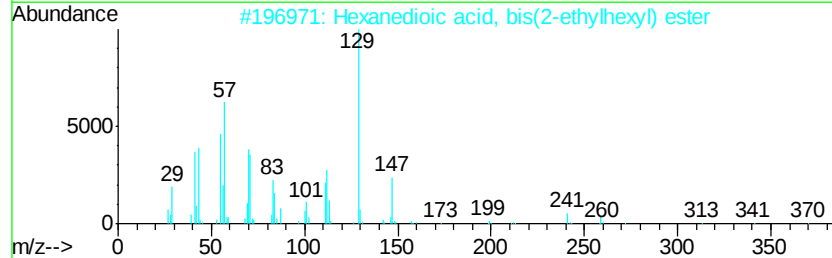
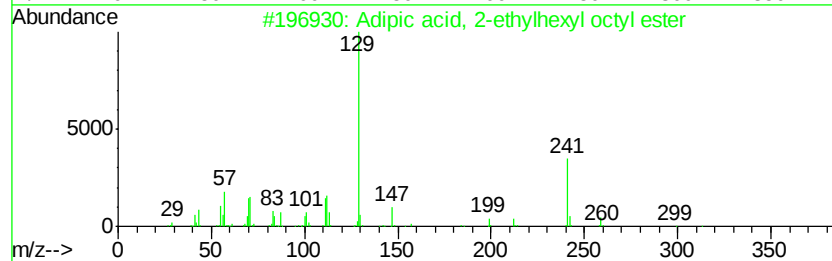
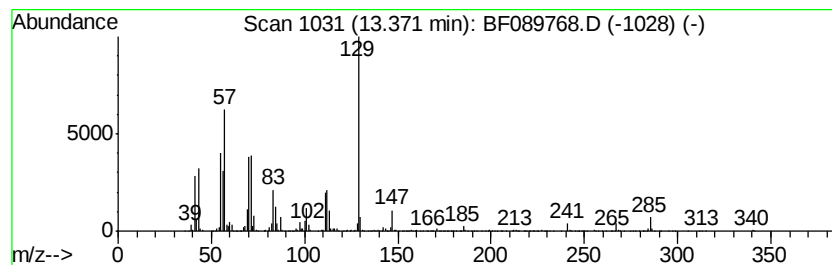
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Adipic acid, 2-ethylhexyl o... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	7.15 ng	2809730	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2		Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
3		Diisooctyl adipate	370	C22H42O4	001330-86-5	83
4		Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	53
5		Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	43



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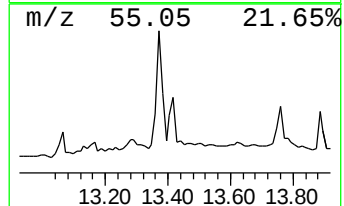
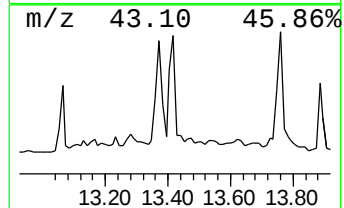
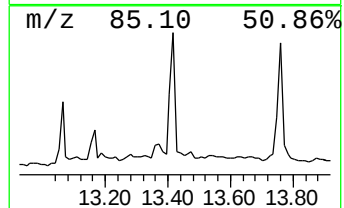
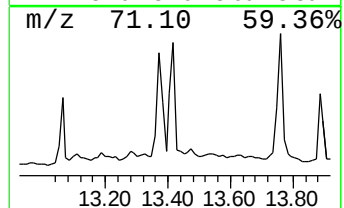
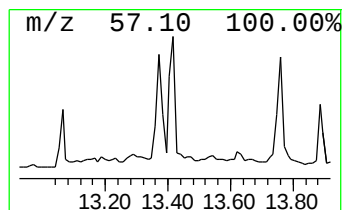
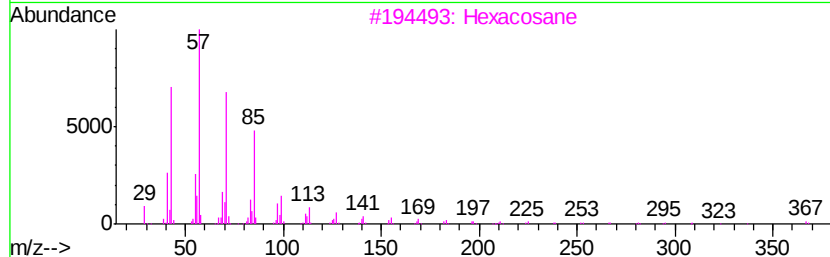
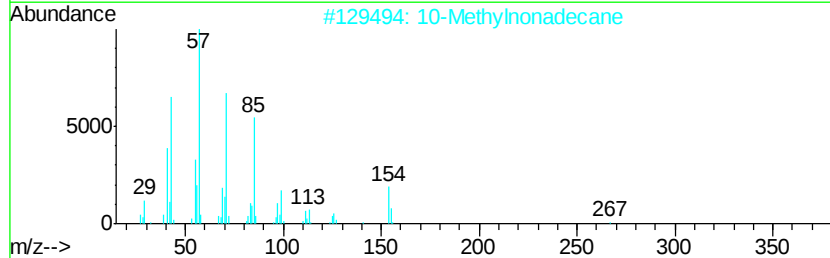
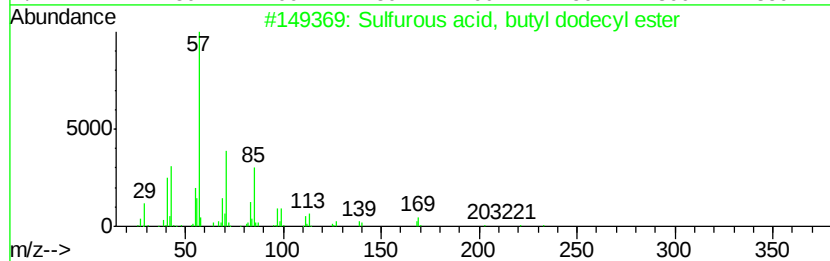
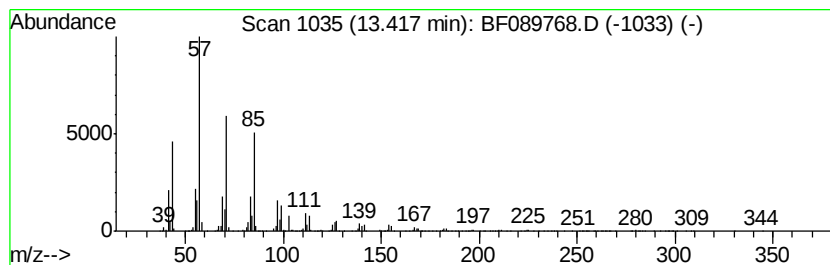
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 Sulfurous acid, butyl dodec... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	3.22 ng	1264760	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
2		10-Methylnonadecane	282	C20H42	056862-62-5	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tetratetracontane	619	C44H90	007098-22-8	86
5		Hexadecane	226	C16H34	000544-76-3	83



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ClientSampleId :
LOCATION-19A

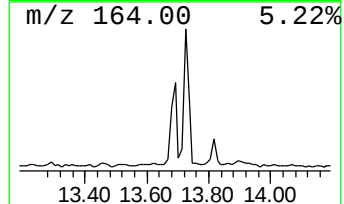
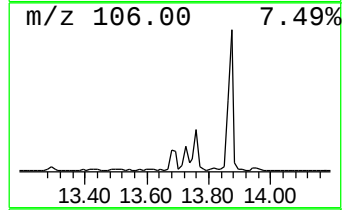
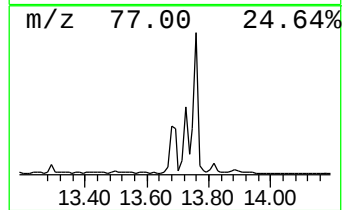
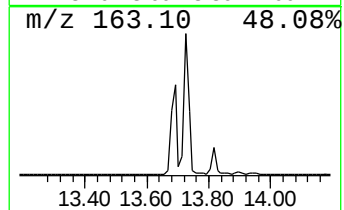
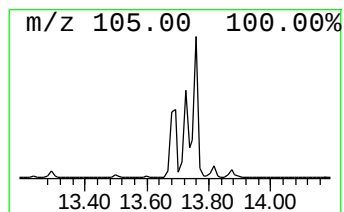
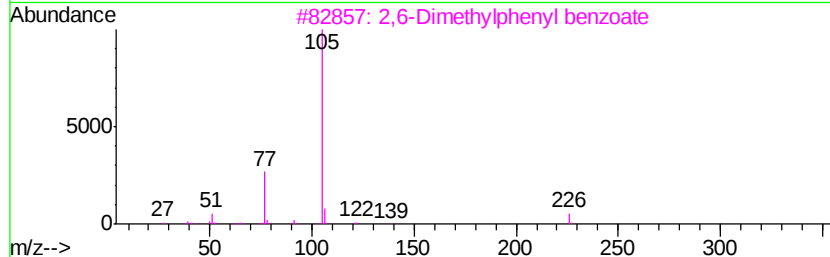
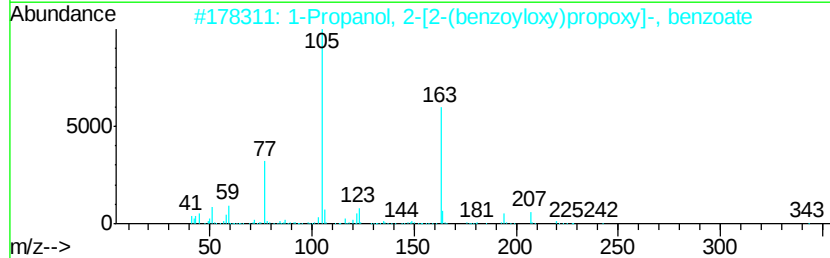
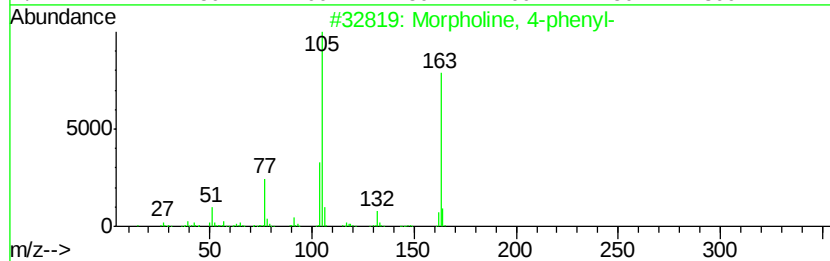
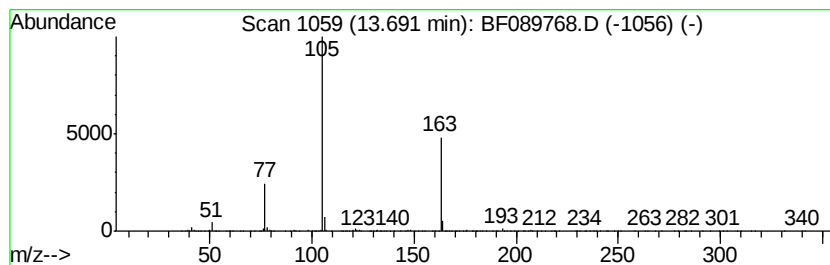
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.69 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	2.21 ng	867395	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	42
2		1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40
3		2,6-Dimethylphenyl benzoate	226	C15H14O2	001871-36-9	38
4		Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	38
5		1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081716\
Data File : BF089768.D
Acq On : 17 Aug 2016 17:40
Operator : UM/SJ
Sample : H4476-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-19A

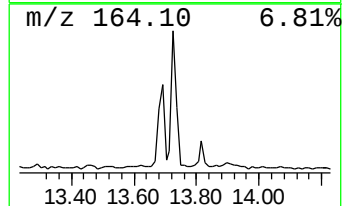
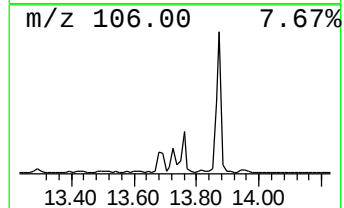
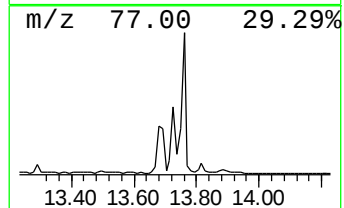
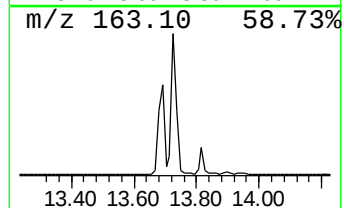
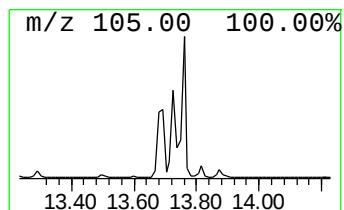
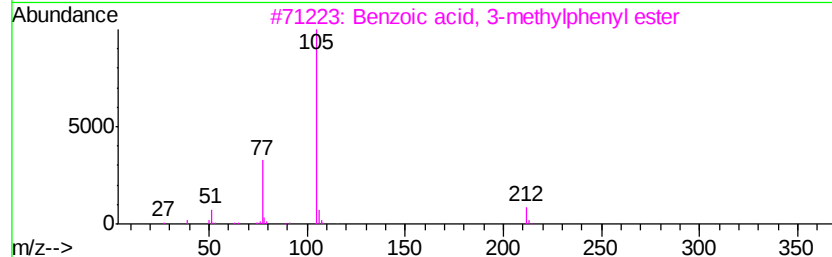
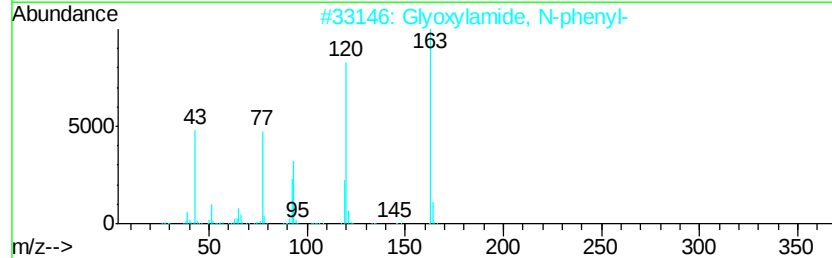
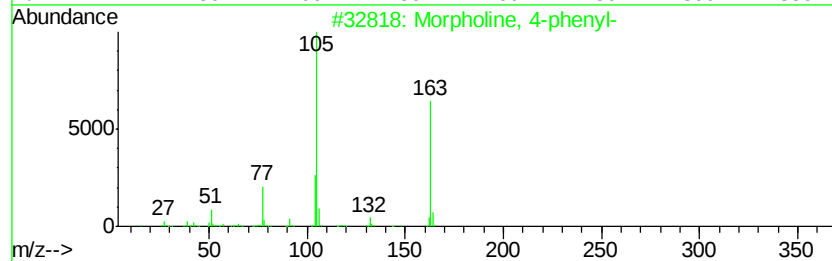
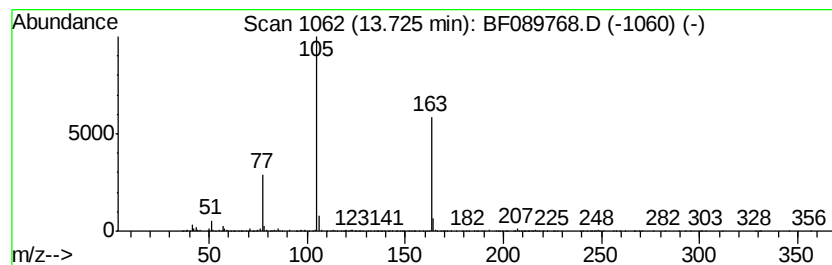
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Morpholine, 4-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.38 ng	934422	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2		Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3		Benzoic acid, 3-methylphenyl ester	212	C14H12O2	1000357-80-0	35
4		N-Benzoyl-N-ethyl-3,4-methylened...	311	C19H21NO3	1000281-43-7	35
5		Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081716\
Data File : BF089768.D
Acq On : 17 Aug 2016 17:40
Operator : UM/SJ
Sample : H4476-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-19A

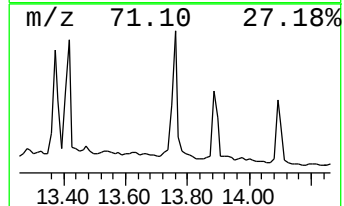
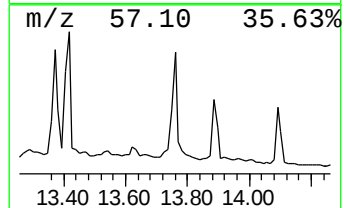
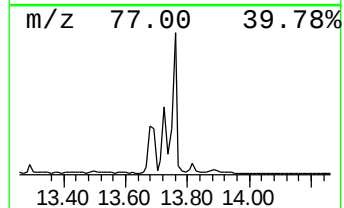
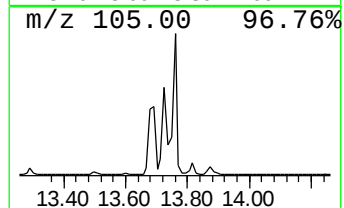
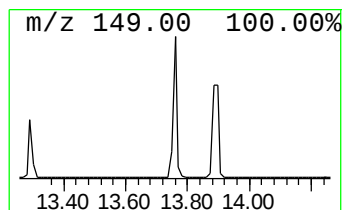
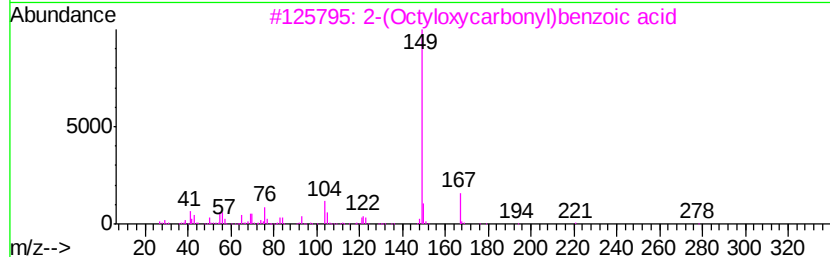
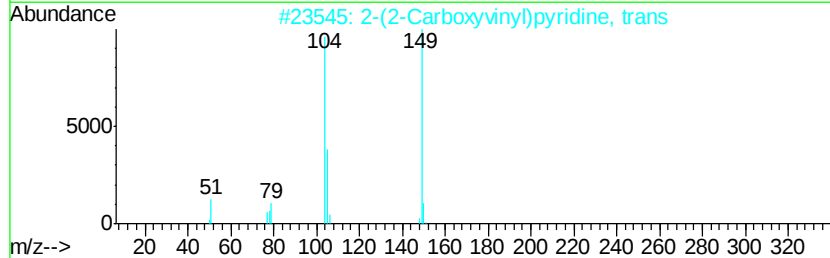
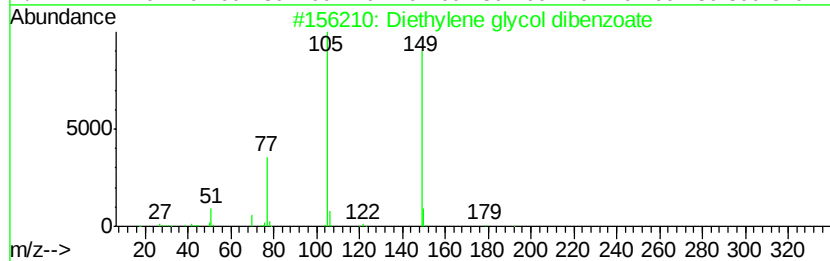
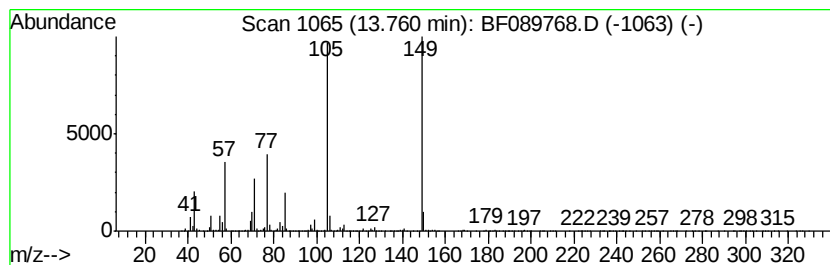
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.29 ng	2472100	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	58
2		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	43
3		2-(Octyloxycarbonyl)benzoic acid	278	C16H22O4	1000373-53-3	38
4		Phthalic acid, 4,4-dimethylpent-...	516	C33H56O4	1000371-12-8	38
5		Phthalic acid, hept-2-yl isobuty...	320	C19H28O4	1000356-97-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081716\
Data File : BF089768.D
Acq On : 17 Aug 2016 17:40
Operator : UM/SJ
Sample : H4476-04
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-19A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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...	4.83	7.9	ng	1406130	1	6.70	3575900	20.0
unknown6.47	6.47	78.3	ng	13994600	1	6.70	3575900	20.0
Octadecanoic acid	12.56	18.3	ng	7180770	5	13.87	7864680	20.0
Adipic acid, 2-et...	13.37	7.2	ng	2809730	5	13.87	7864680	20.0
Sulfurous acid, b...	13.42	3.2	ng	1264760	5	13.87	7864680	20.0
unknown13.69	13.69	2.2	ng	867395	5	13.87	7864680	20.0
Morpholine, 4-phe...	13.73	2.4	ng	934422	5	13.87	7864680	20.0
Diethylene glycol...	13.76	6.3	ng	2472100	5	13.87	7864680	20.0