

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
 Data File : BF091980.D
 Acq On : 27 Dec 2016 21:04
 Operator : UM/SJ
 Sample : H6244-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LIP-22

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-BF122116.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	4.876	242	244	259	rVB	689534	1069766	14.67%	2.086%
2	5.344	283	285	288	rBV	2411565	3483232	47.77%	6.793%
3	6.407	375	378	384	rVB	1542892	2450344	33.60%	4.779%
4	6.510	384	387	389	rBV	6007552	6104516	83.72%	11.905%
5	6.670	398	401	404	rBV	52239	78855	1.08%	0.154%
6	6.727	404	406	408	rBV	1626131	1433400	19.66%	2.795%
7	6.887	417	420	422	rBV	4856868	5259921	72.14%	10.258%
8	7.299	453	456	458	rBV	3489867	3697255	50.70%	7.210%
9	7.756	493	496	500	rBV3	55029	115545	1.58%	0.225%
10	7.950	508	513	516	rBV4	82437	191145	2.62%	0.373%
11	8.019	516	519	521	rBV	1740070	1799058	24.67%	3.508%
12	8.259	534	540	542	rBV6	70015	173235	2.38%	0.338%
13	8.556	564	566	567	rBV	56115	76798	1.05%	0.150%
14	8.762	582	584	587	rVV3	43533	93981	1.29%	0.183%
15	8.853	587	592	594	rVV6	43530	162259	2.23%	0.316%
16	8.990	601	604	606	rBV4	58679	153913	2.11%	0.300%
17	9.105	610	614	616	rVB	5508862	7291761	100.00%	14.220%
18	9.287	628	630	632	rVB2	57098	75309	1.03%	0.147%
19	9.425	640	642	645	rBV2	76547	168771	2.31%	0.329%
20	9.493	646	648	653	rVB	213778	304081	4.17%	0.593%
21	9.619	658	659	662	rBV2	54841	73921	1.01%	0.144%
22	9.710	665	667	670	rBV4	51060	111954	1.54%	0.218%
23	9.768	670	672	675	rBV	1971775	1833305	25.14%	3.575%
24	10.202	708	710	714	rVB3	97892	146456	2.01%	0.286%
25	10.568	739	742	744	rVV	3704008	3868529	53.05%	7.544%
26	10.682	750	752	755	rVB3	67381	86817	1.19%	0.169%
27	11.128	789	791	793	rVB	130610	135701	1.86%	0.265%
28	11.253	799	802	804	rVB	1931965	1653512	22.68%	3.225%
29	11.608	831	833	835	rVB	125145	122996	1.69%	0.240%
30	11.825	849	852	862	rVB2	113991	360770	4.95%	0.704%
31	12.602	917	920	922	rBV3	55040	132907	1.82%	0.259%
32	12.842	938	941	944	rBV	4643956	5526123	75.79%	10.777%
33	13.196	971	972	978	rBV5	43156	147832	2.03%	0.288%
34	13.436	991	993	996	rVB	338667	339201	4.65%	0.661%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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35	13.894	1030	1033	1035	rBV	1130718	1351892	18.54%	2.636%
36	15.288	1152	1155	1158	rBV	897053	1072804	14.71%	2.092%
37	17.265	1324	1328	1331	rBV5	36404	130038	1.78%	0.254%

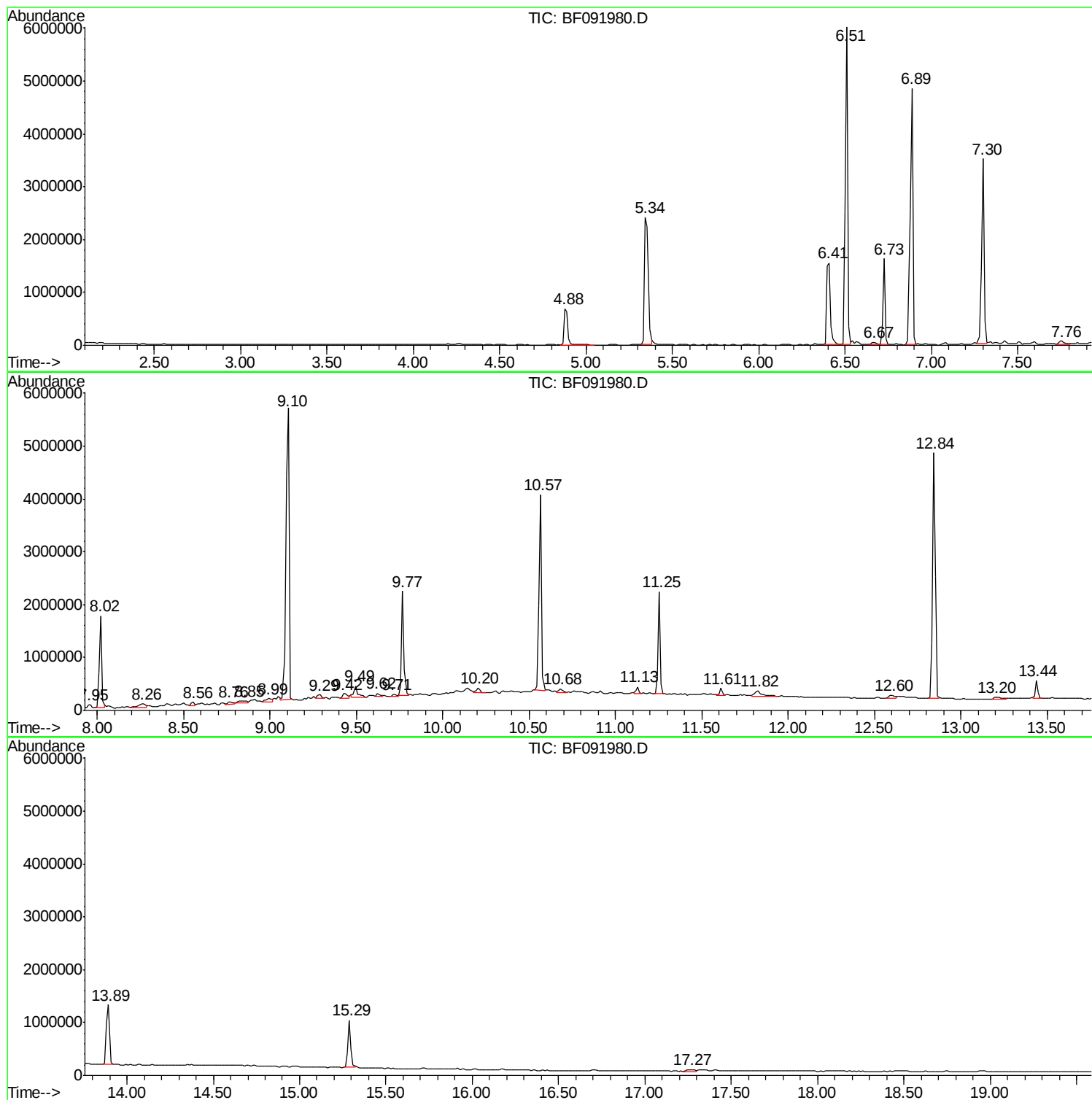
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : UM/SJ
Sample : H6244-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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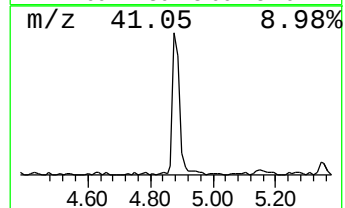
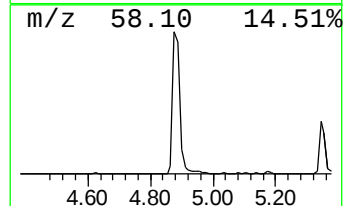
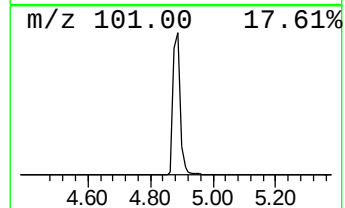
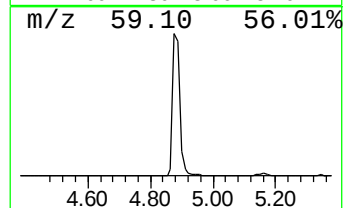
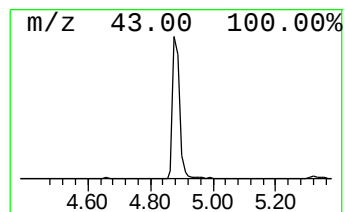
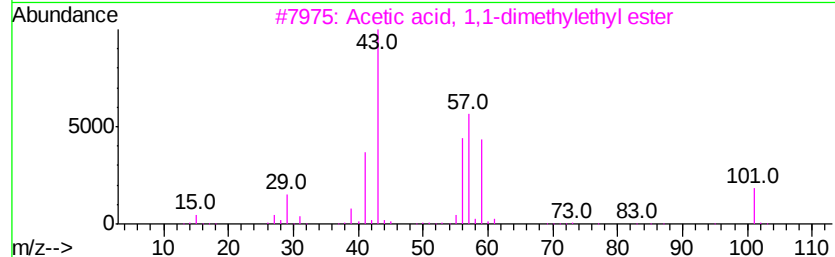
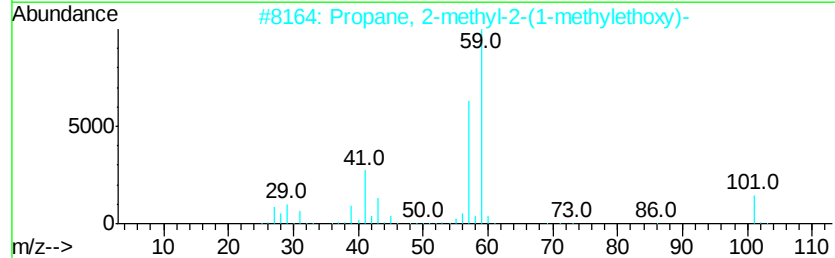
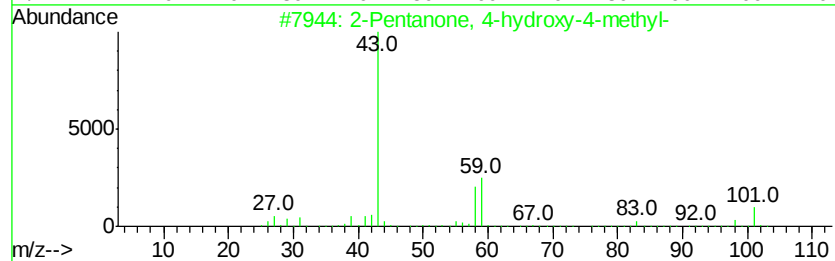
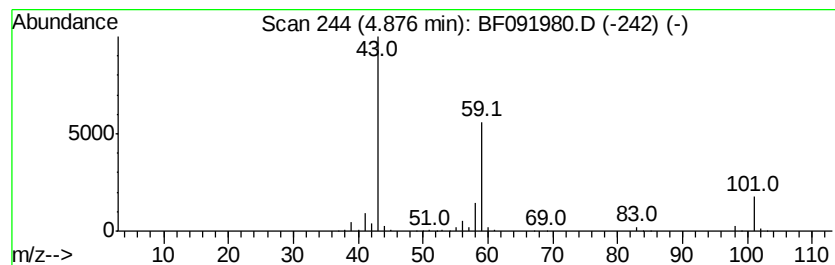
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.88	14.93 ng	1069770	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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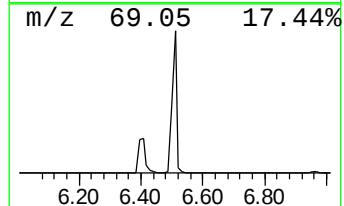
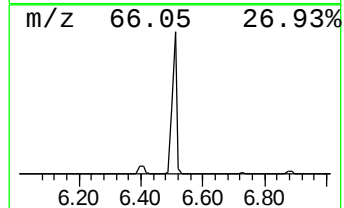
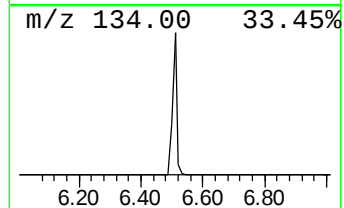
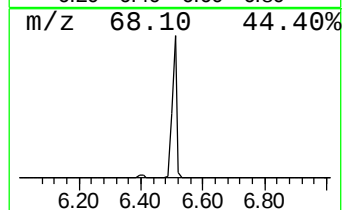
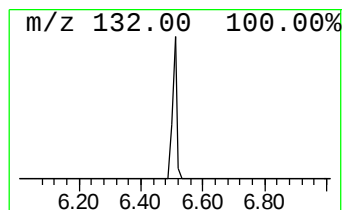
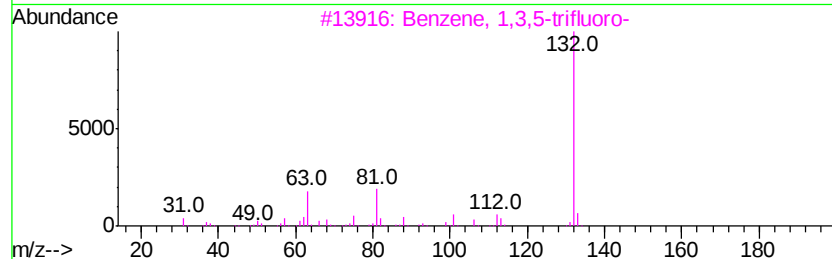
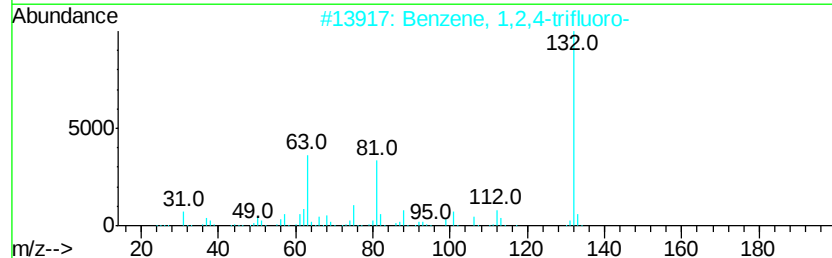
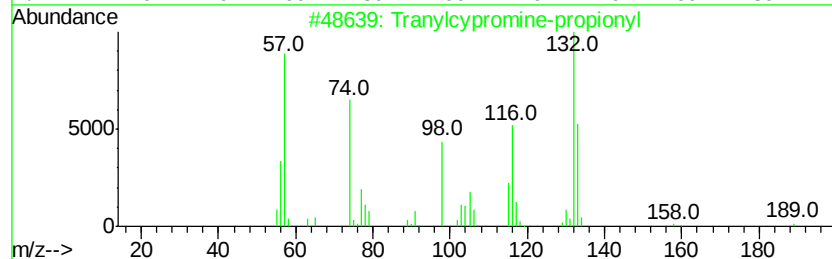
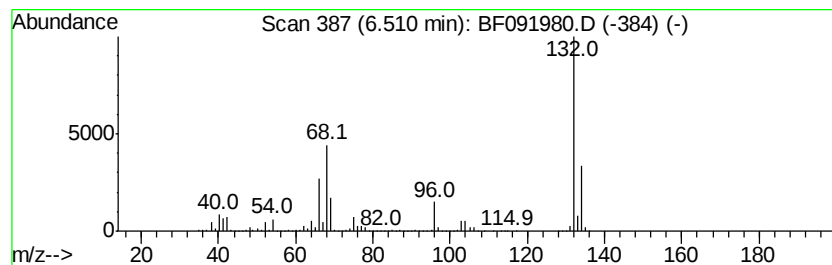
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	85.18 ng	6104520	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
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		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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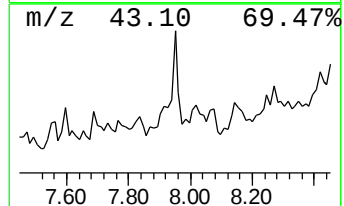
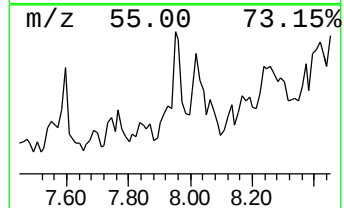
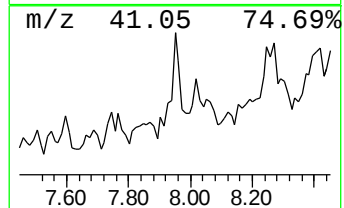
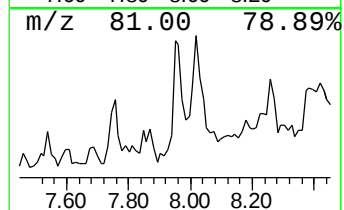
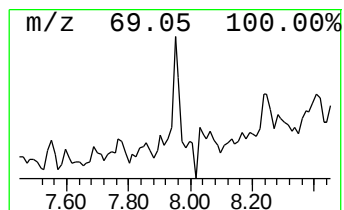
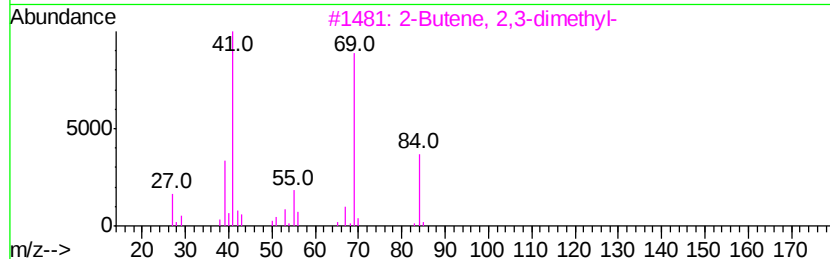
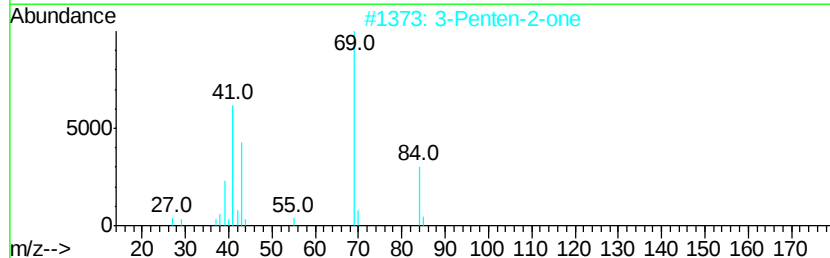
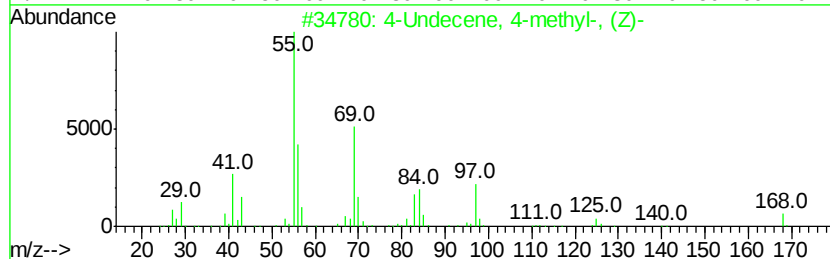
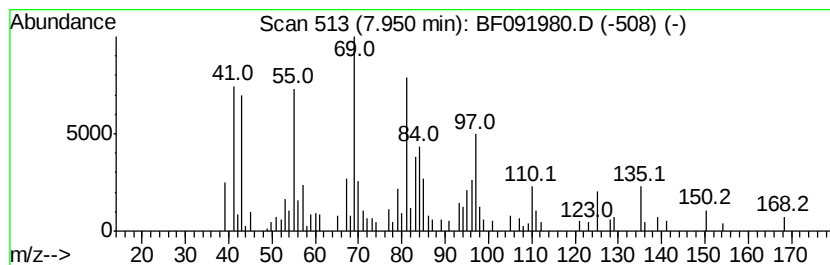
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.95 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.95	2.12 ng	191145	Napthalene-d8	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4	Undecene, 4-methyl-, (Z)-	168	C12H24	074630-57-2	45
2	3	Penten-2-one	84	C5H8O	000625-33-2	25
3	2	Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	25
4	2,6,10	Dodecatrienal, 3,7,11-tri...	220	C15H24O	000502-67-0	22
5	Methyl ethyl	cyclopentene	110	C8H14	019780-56-4	20



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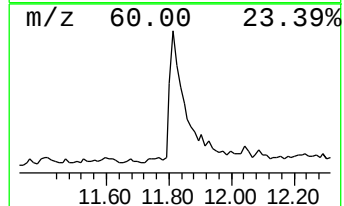
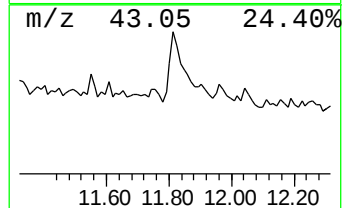
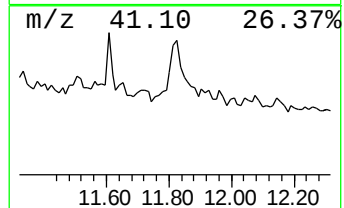
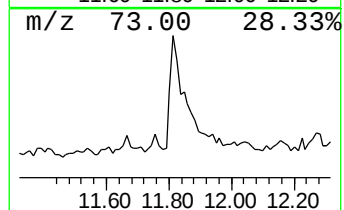
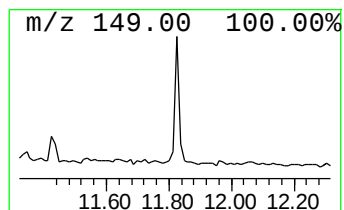
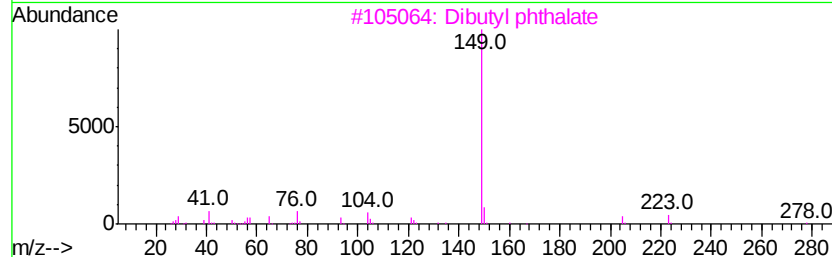
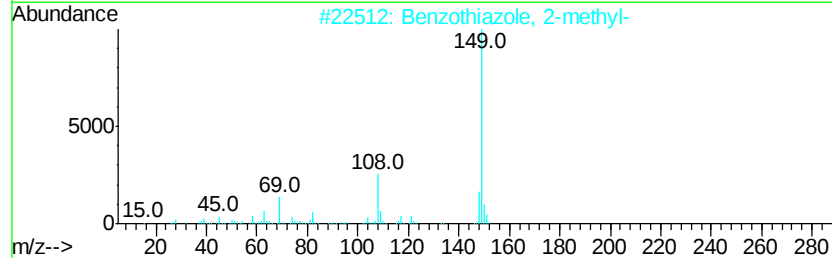
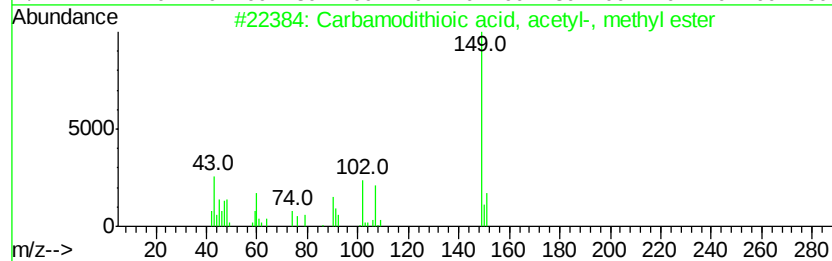
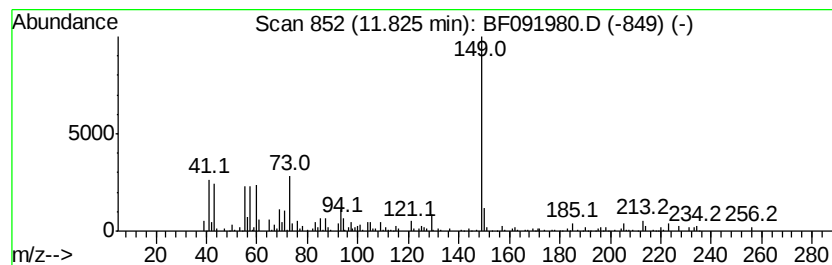
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Carbamodithioic acid, acety... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	4.36 ng	360770	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbamodithioic acid, acetyl-, m...	149	C4H7NOS2	016696-88-1	53
2		Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	49
3		Dibutyl phthalate	278	C16H22O4	000084-74-2	47
4		Pyrindine, pentamethyl-	149	C10H15N	003748-83-2	47
5		1,2-Benzenedicarboxylic acid, di...	334	C20H30O4	000084-75-3	47



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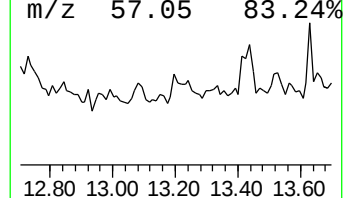
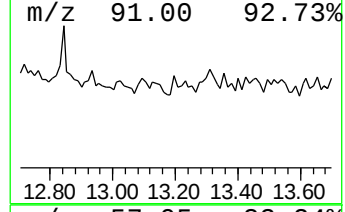
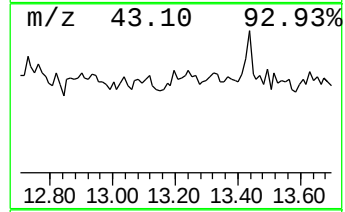
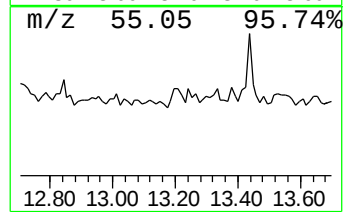
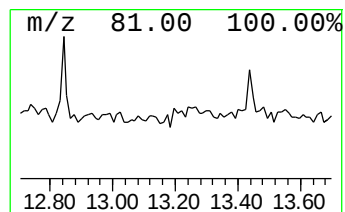
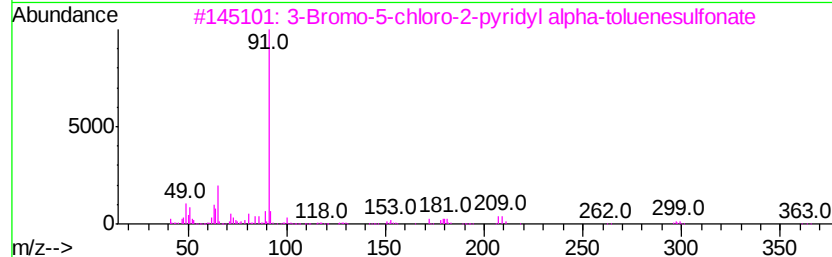
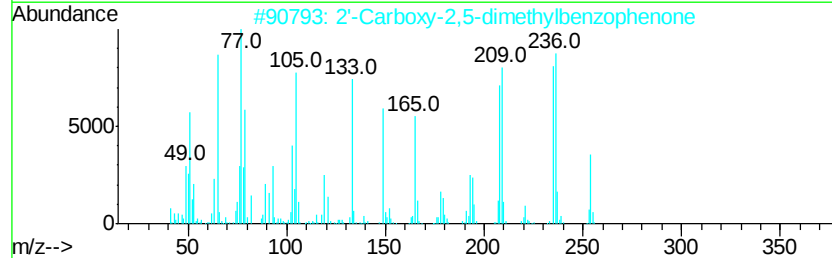
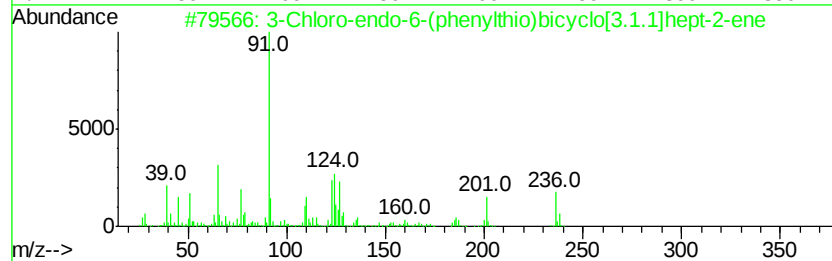
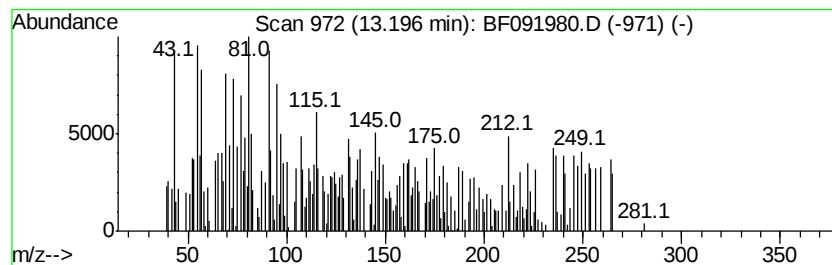
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.20 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	2.19 ng	147832	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-endo-6-(phenylthio)bicyclo[3.1.1]hept-2-ene	236	C13H13ClS	102870-57-5	38
2		2'-Carboxy-2,5-dimethylbenzophenone	254	C16H14O3	060288-22-4	32
3		3-Bromo-5-chloro-2-pyridyl alpha-toluenesulfonate	361	C12H9BrClN03S	058236-60-5	27
4		Benzaldehyde, 2-(phenylmethoxy)-	212	C14H12O2	005896-17-3	25
5		Benzene, 1,3-dimethyl-2-(phenylmethyl)-	212	C15H16O	019578-74-6	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091980.D
Acq On : 27 Dec 2016 21:04
Operator : UM/SJ
Sample : H6244-04
Misc :
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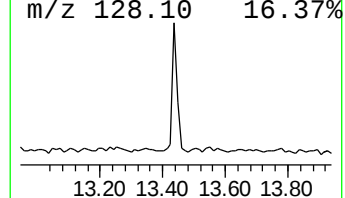
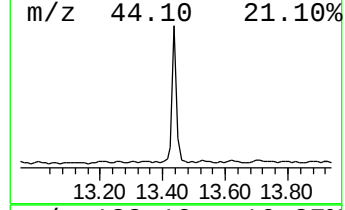
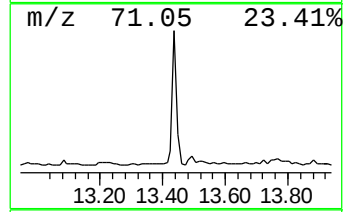
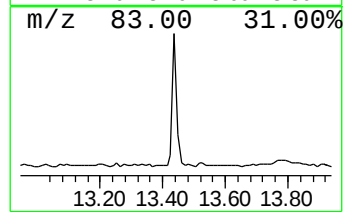
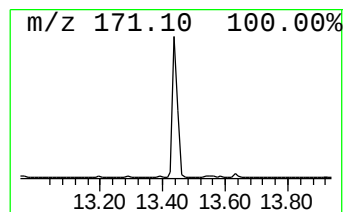
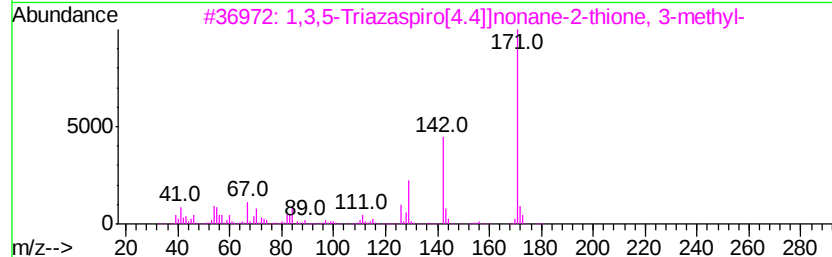
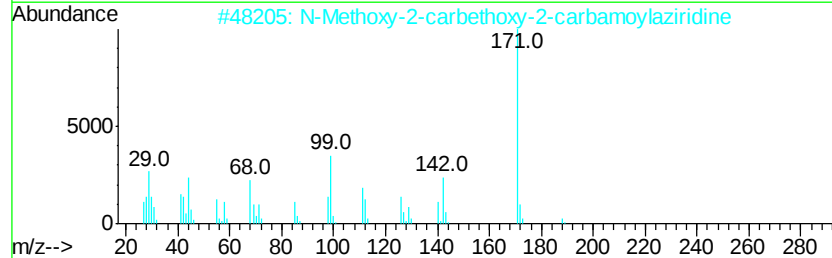
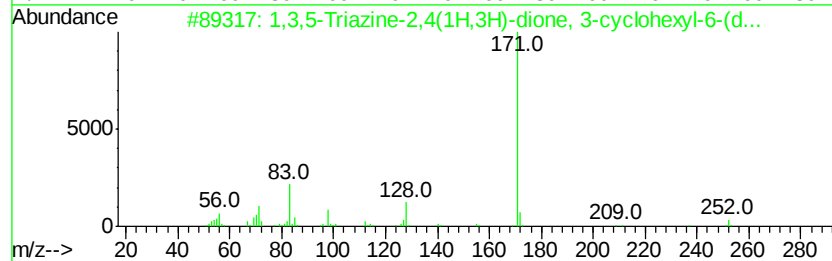
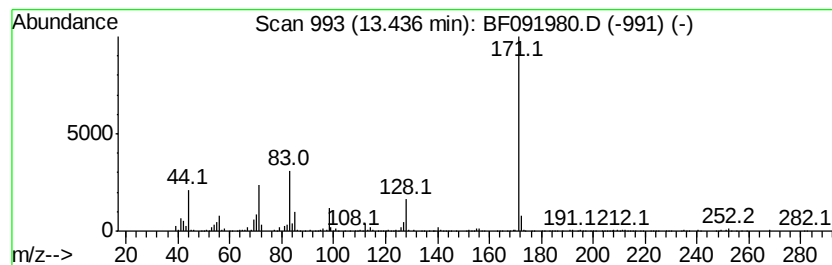
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BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.44	5.02 ng	339201	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	86
2	N-Methoxy-2-carbethoxy-2-carbamo...	188	C7H12N2O4	063859-03-0	42
3	1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	38
4	4-Pyridinol, 2-phenyl-	171	C11H9NO	1000253-54-5	32
5	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122716\
Data File : BF091980.D
Acq On : 27 Dec 2016 21:04
Operator : UM/SJ
Sample : H6244-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

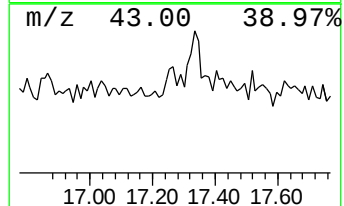
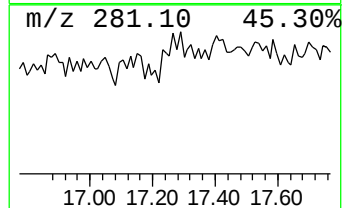
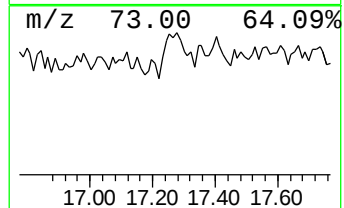
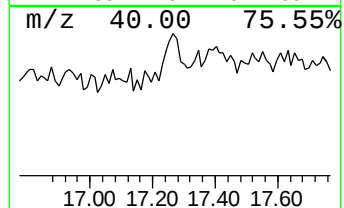
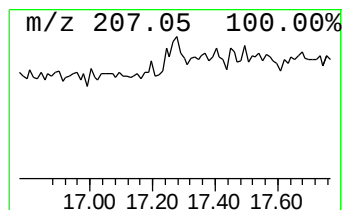
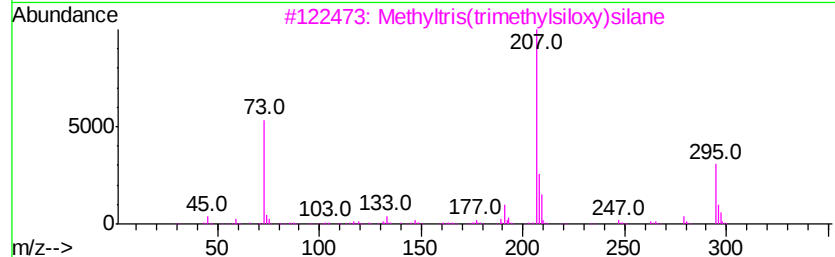
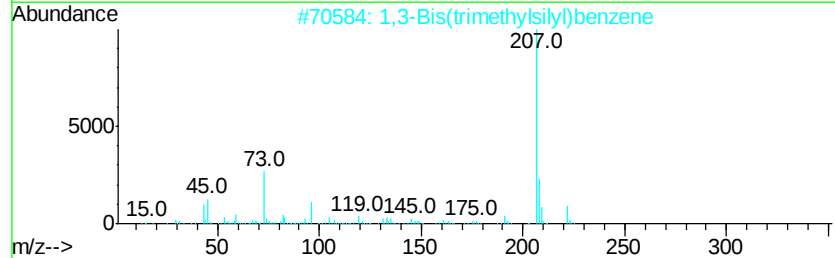
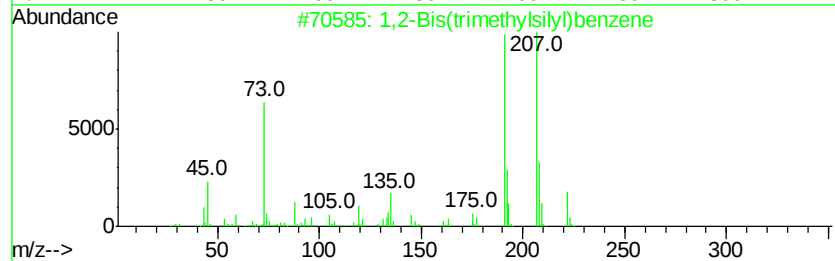
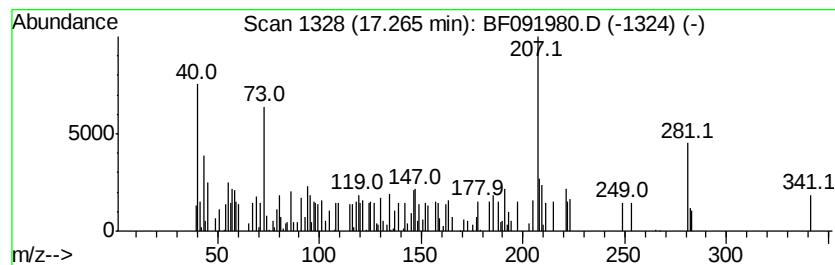
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,2-Bis(trimethylsilyl)benzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	2.42 ng	130038	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	50
2		1,3-Bis(trimethylsilyl)benzene	222	C12H22Si2	002060-89-1	38
3		Methyltris(trimethylsiloxy)silane	310	C10H30O3Si4	017928-28-8	32
4		2-Methyl-7-phenylindole	207	C15H13N	001140-08-5	30
5		4-Quinolinecarboxylic acid, 2-ch...	207	C10H6ClN02	005467-57-2	30



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Sample : H6244-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	14.9	ng	1069770	1	6.73	1433400	20.0
unknown6.51	6.51	85.2	ng	6104520	1	6.73	1433400	20.0
unknown7.95	7.95	2.1	ng	191145	2	8.02	1799060	20.0
Carbamodithioic a...	11.82	4.4	ng	360770	4	11.25	1653510	20.0
unknown13.20	13.20	2.2	ng	147832	5	13.89	1351890	20.0
1,3,5-Triazine-2,...	13.44	5.0	ng	339201	5	13.89	1351890	20.0
1,2-Bis(trimethyl...	17.27	2.4	ng	130038	6	15.29	1072800	20.0