

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030215\
 Data File : BF077535.D
 Acq On : 2 Mar 2015 21:18
 Operator : TP/IZ
 Sample : G1399-09
 Misc : S
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB3

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.184	22	26	29	rVB	743002	1324234	24.88%	4.295%
2	1.413	44	46	49	rBV	4366494	5322164	100.00%	17.262%
3	1.550	54	58	61	rVB	1033166	1679186	31.55%	5.446%
4	1.721	71	73	76	rVB	282205	319508	6.00%	1.036%
5	1.847	80	84	94	rVB2	97478	178482	3.35%	0.579%
6	5.036	361	363	374	rVB	270769	325376	6.11%	1.055%
7	5.550	406	408	411	rBV	1330859	1490025	28.00%	4.833%
8	6.819	517	519	522	rBV	1407063	1432926	26.92%	4.648%
9	6.967	530	532	535	rBV	1282883	1606011	30.18%	5.209%
10	7.265	555	558	560	rVB	509900	518765	9.75%	1.683%
11	7.447	572	574	577	rVB	1406451	1249451	23.48%	4.052%
12	7.950	616	618	621	rBV	1004110	906790	17.04%	2.941%
13	8.842	693	696	698	rBV	640630	721006	13.55%	2.338%
14	10.179	811	813	816	rBV	1694939	1827102	34.33%	5.926%
15	10.682	855	857	860	rBV	56553	73585	1.38%	0.239%
16	11.014	884	886	888	rBV	867446	848635	15.95%	2.752%
17	11.916	962	965	967	rBV	82599	105796	1.99%	0.343%
18	11.985	969	971	974	rBV2	921951	1164602	21.88%	3.777%
19	12.854	1044	1047	1049	rBV	946655	992263	18.64%	3.218%
20	12.888	1049	1050	1052	rVV	200373	142495	2.68%	0.462%
21	12.945	1053	1055	1057	rVB	78983	76658	1.44%	0.249%
22	13.620	1112	1114	1115	rBV	76784	93162	1.75%	0.302%
23	13.860	1133	1135	1140	rVB2	40006	75915	1.43%	0.246%
24	14.362	1176	1179	1181	rBV	528293	525226	9.87%	1.704%
25	14.637	1200	1203	1205	rBV	506986	603518	11.34%	1.957%
26	14.854	1219	1222	1224	rBV	1956605	2152652	40.45%	6.982%
27	15.060	1238	1240	1242	rVB	67470	82495	1.55%	0.268%
28	15.185	1249	1251	1253	rBV	79814	88484	1.66%	0.287%
29	15.825	1304	1307	1309	rBV	71985	119200	2.24%	0.387%
30	16.020	1321	1324	1330	rBV2	132378	226426	4.25%	0.734%
31	16.145	1331	1335	1337	rVV2	1109982	1552298	29.17%	5.035%
32	16.180	1337	1338	1343	rVB2	246687	253588	4.76%	0.822%
33	16.648	1376	1379	1381	rBV	68823	107712	2.02%	0.349%
34	17.437	1445	1448	1453	rBV	267578	608610	11.44%	1.974%

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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: CENTROID

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.563	1457	1459	1460	rBV	64190	80335	1.51%	0.261%
36	17.757	1474	1476	1479	rBV	157578	213714	4.02%	0.693%
37	17.826	1479	1482	1484	rBV	236106	306351	5.76%	0.994%
38	17.894	1485	1488	1490	rBV	672738	1015112	19.07%	3.292%
39	19.346	1612	1615	1619	rVB2	108442	235225	4.42%	0.763%
40	19.769	1650	1652	1656	rVB	96205	186909	3.51%	0.606%

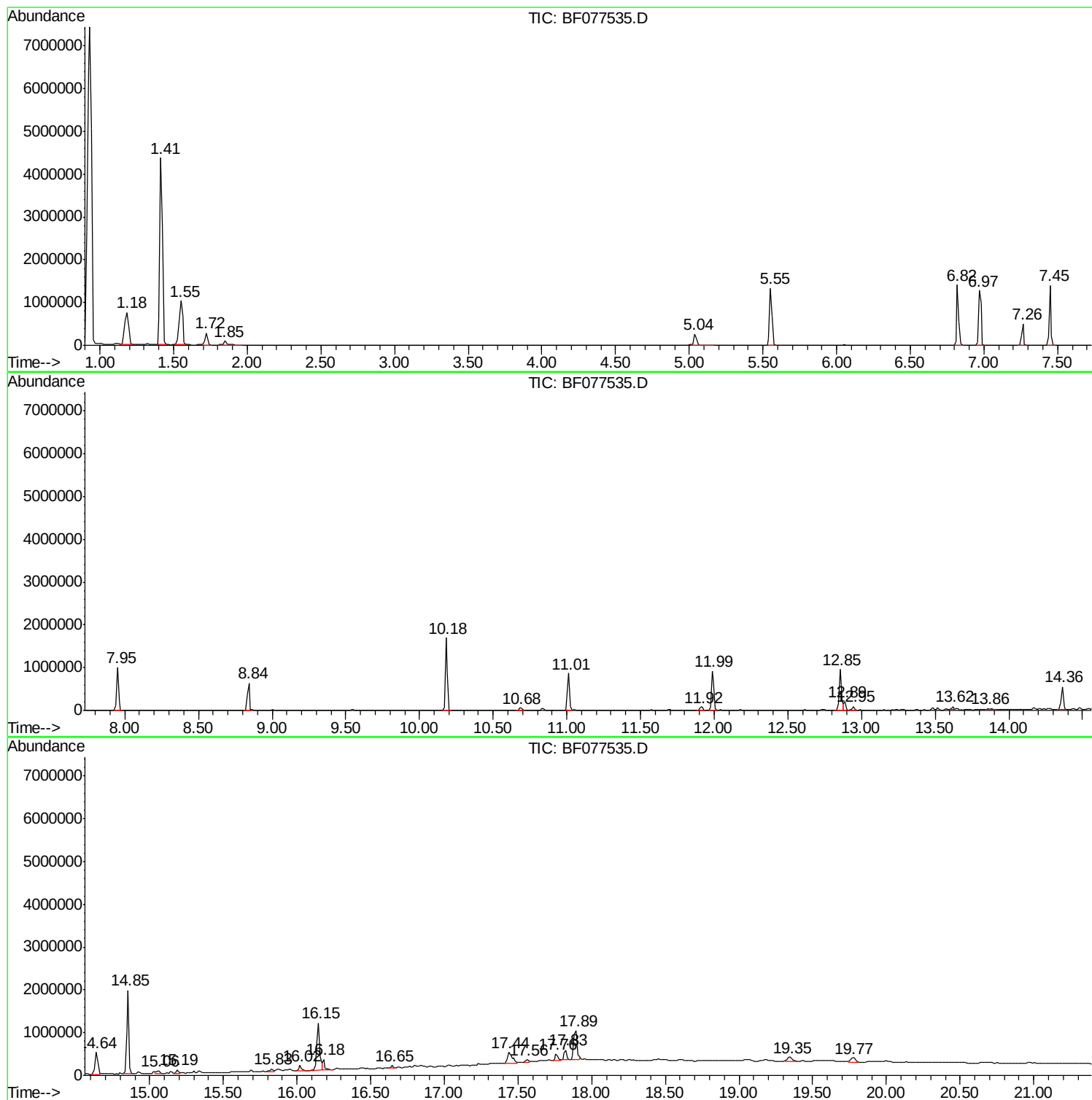
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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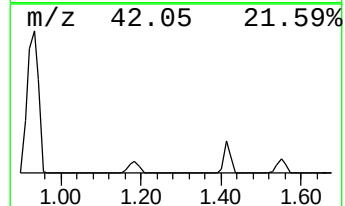
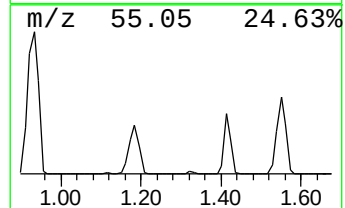
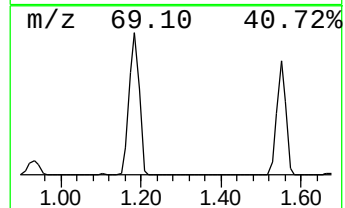
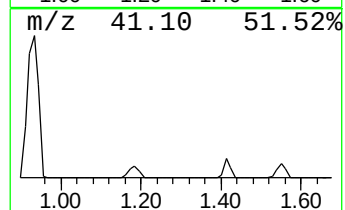
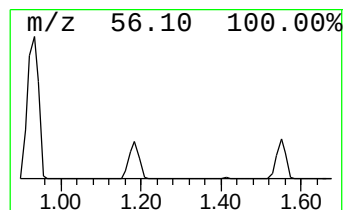
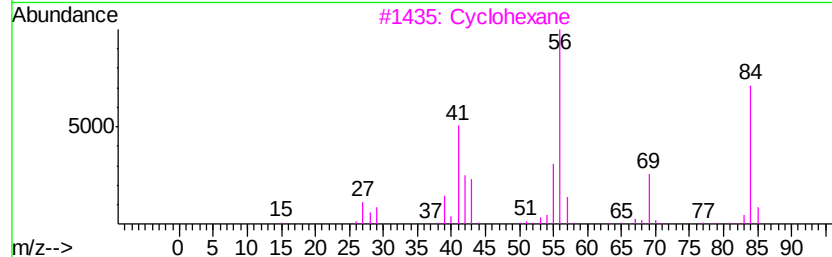
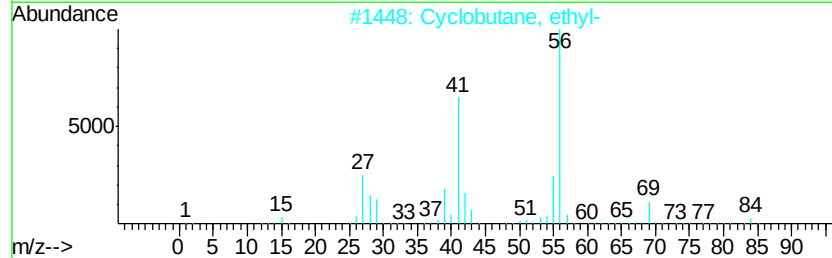
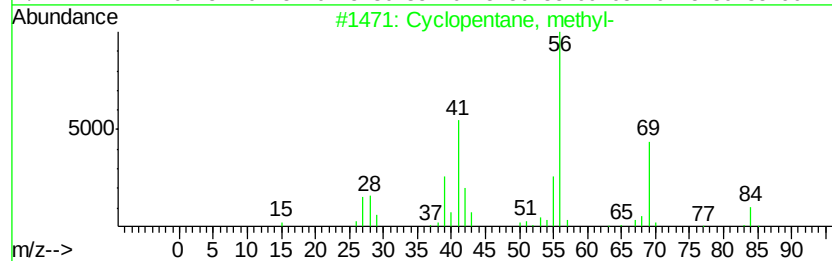
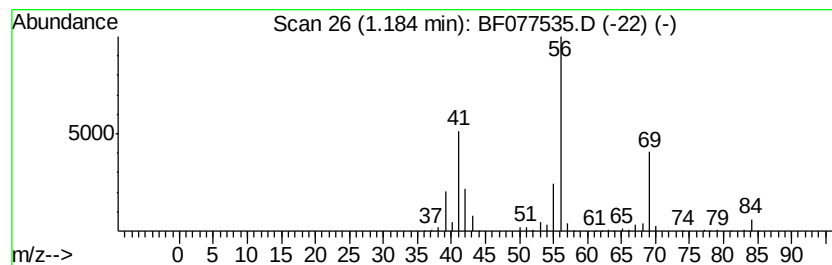
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.18	51.05 ng	1324230	1,4-Dichlorobenzene-d4	7.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	Cyclohexane	84	C6H12	000110-82-7	64
4	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47



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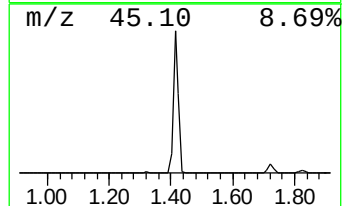
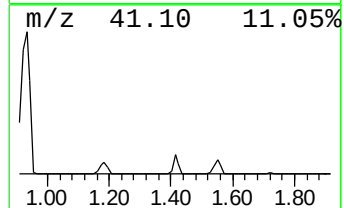
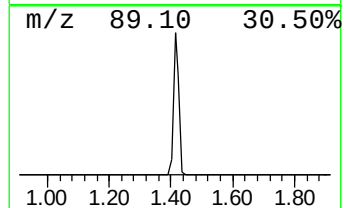
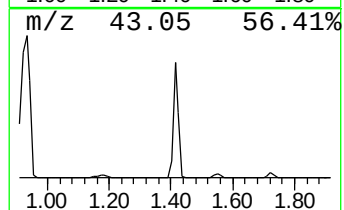
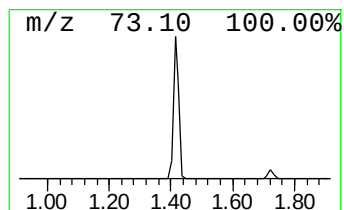
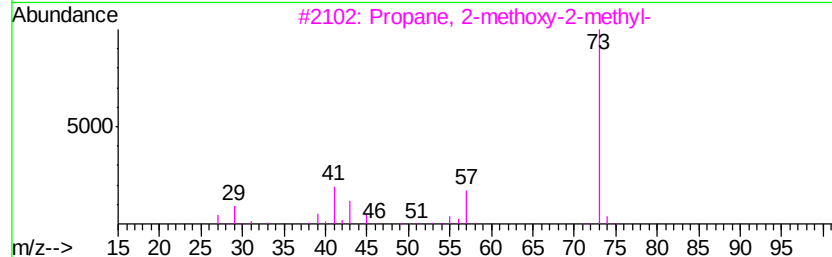
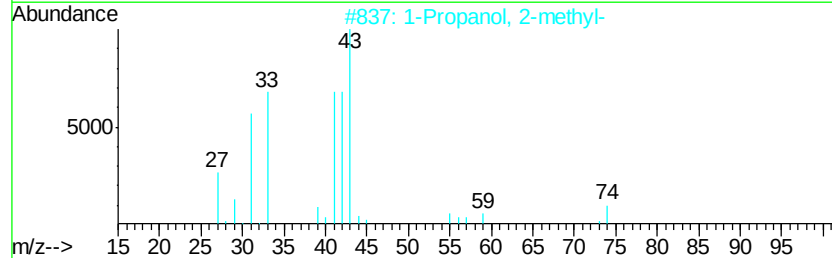
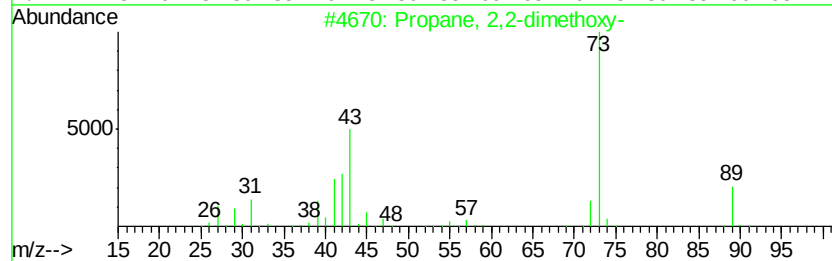
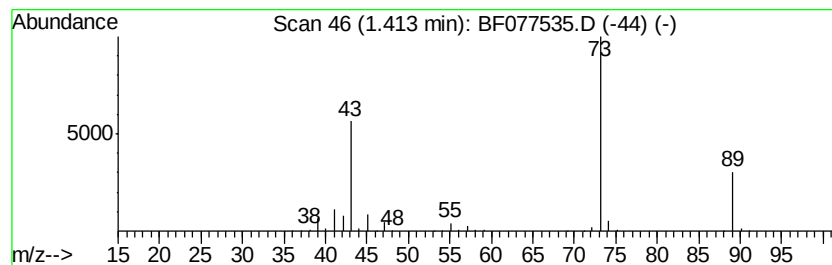
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.41	205.19 ng	5322160	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9



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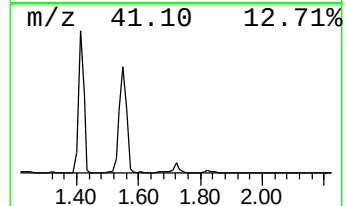
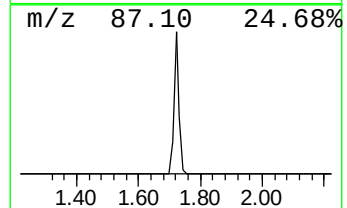
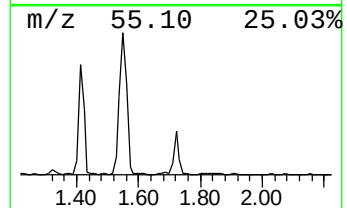
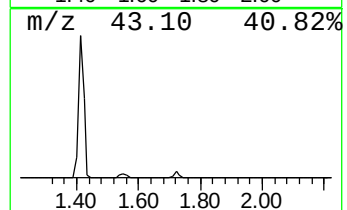
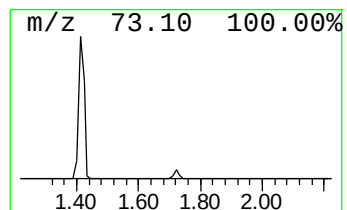
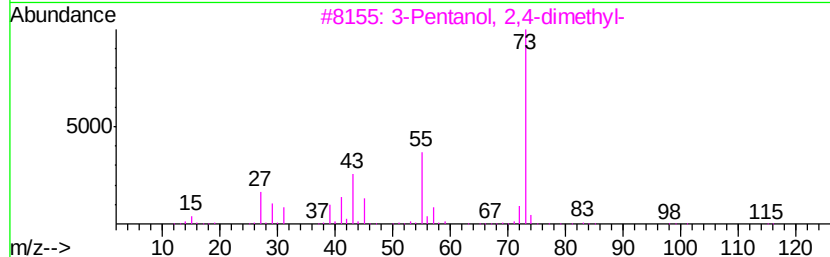
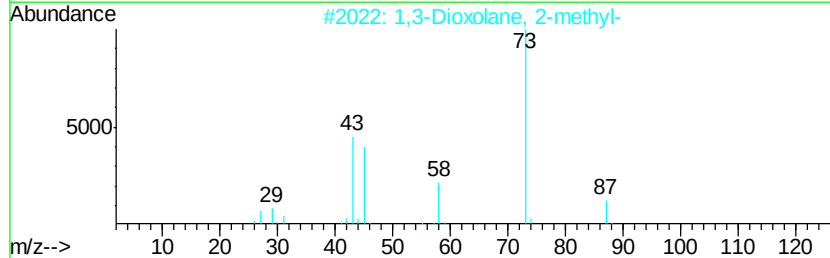
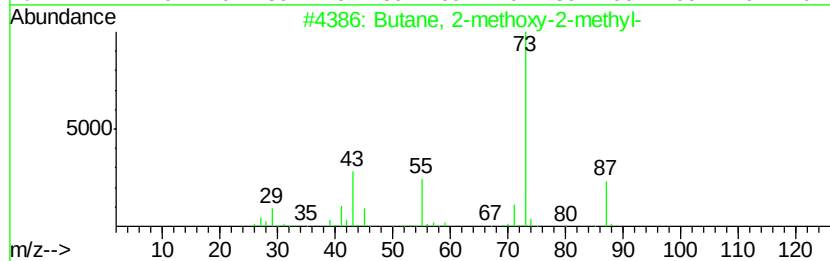
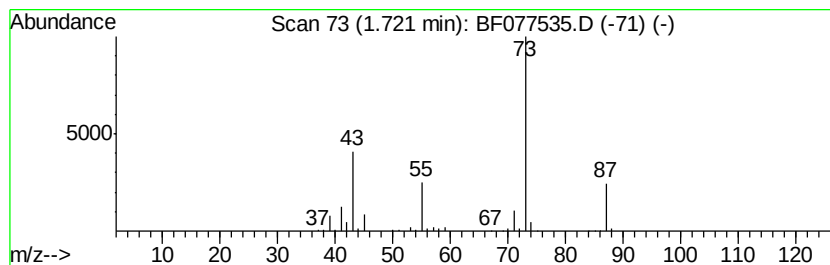
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.72	12.32 ng	319508	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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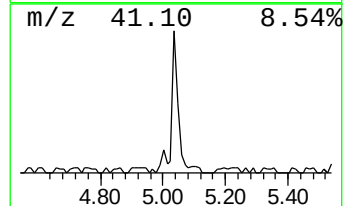
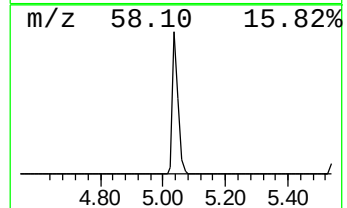
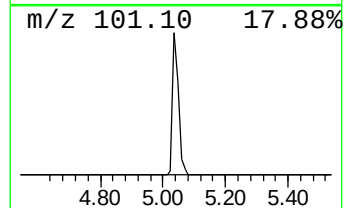
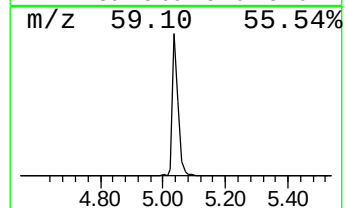
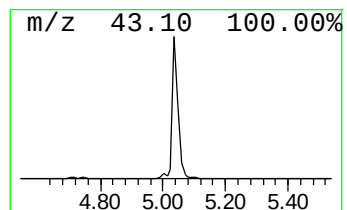
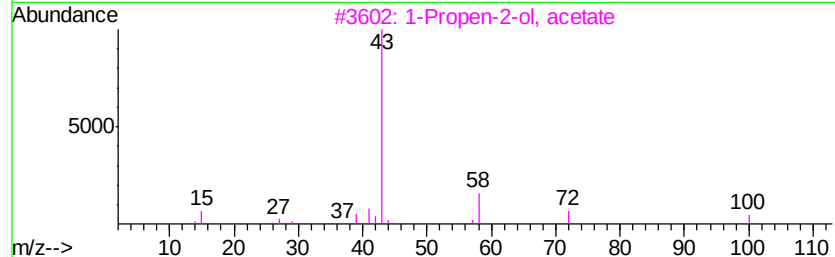
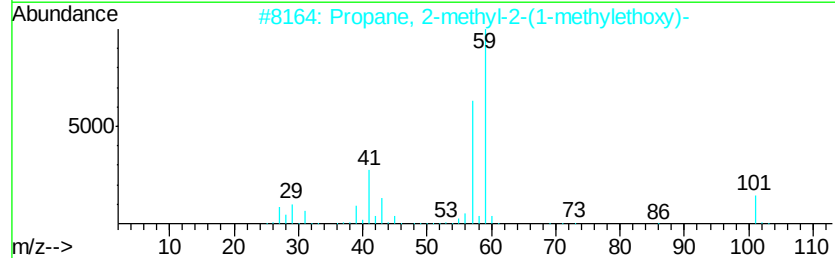
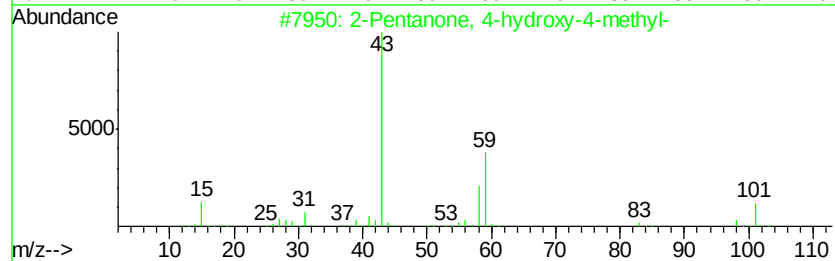
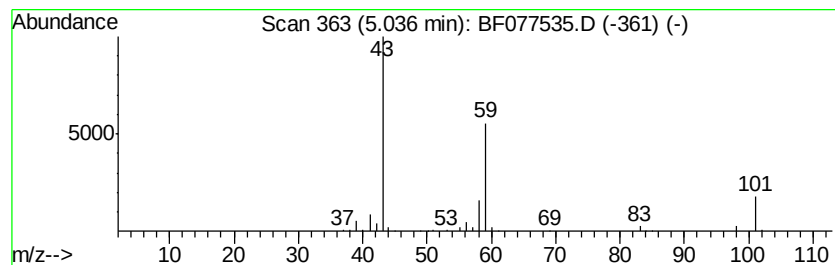
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	12.54 ng	325376	1,4-Dichlorobenzene-d4	7.26

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		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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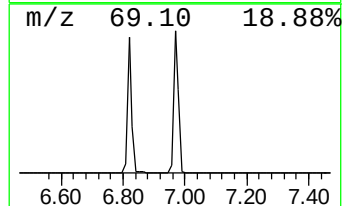
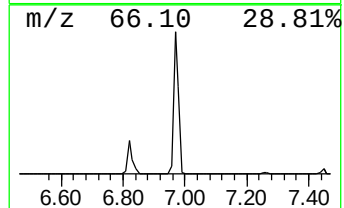
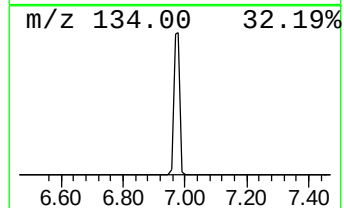
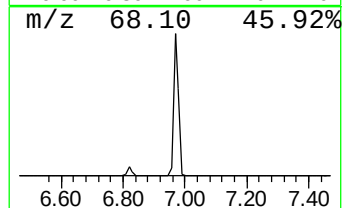
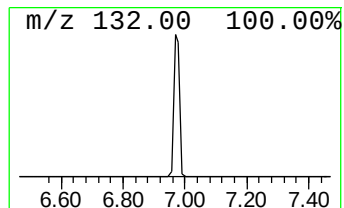
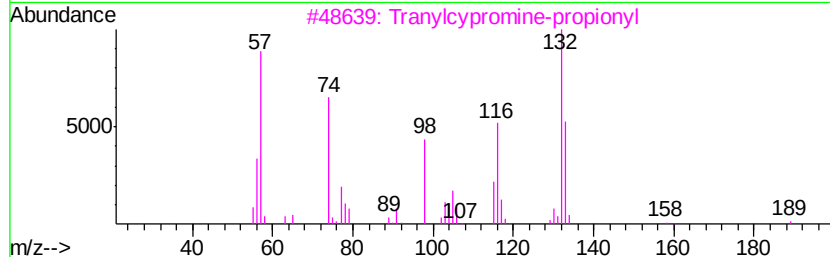
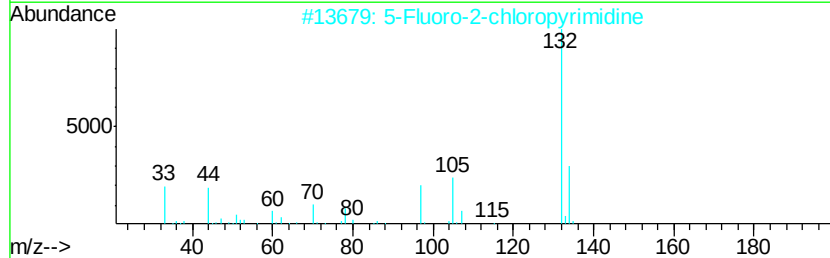
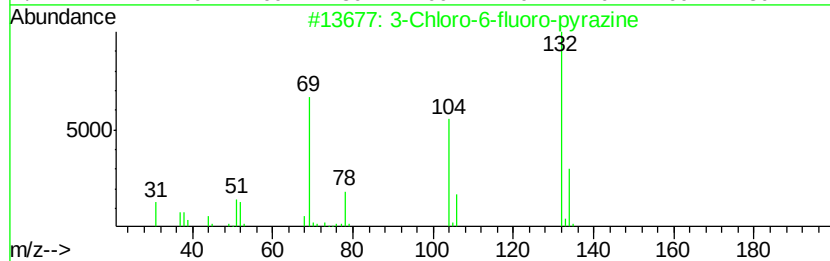
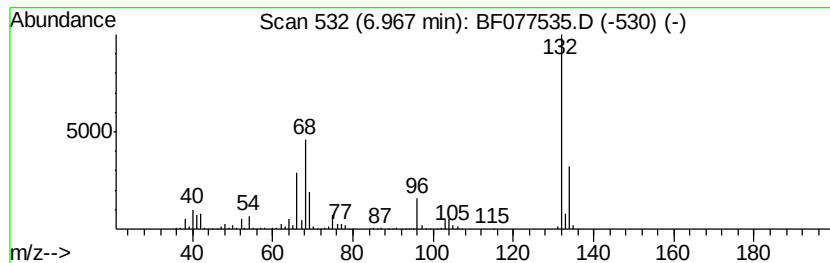
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown6.97 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	61.92 ng	1606010	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030215\
Data File : BF077535.D
Acq On : 2 Mar 2015 21:18
Operator : TP/IZ
Sample : G1399-09
Misc : S
ALS Vial : 16 Sample Multiplier: 1

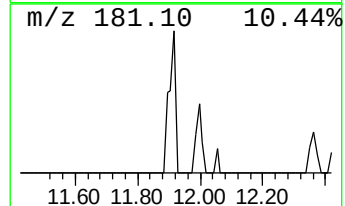
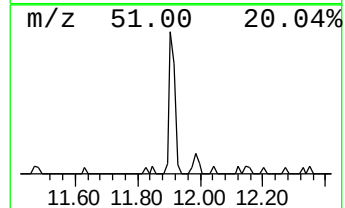
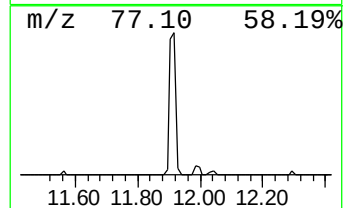
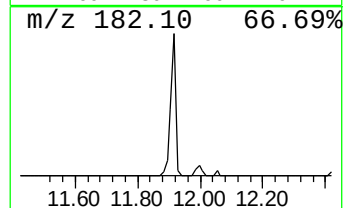
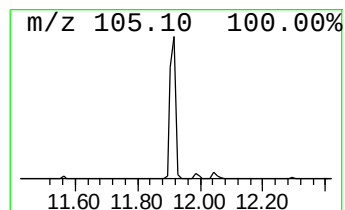
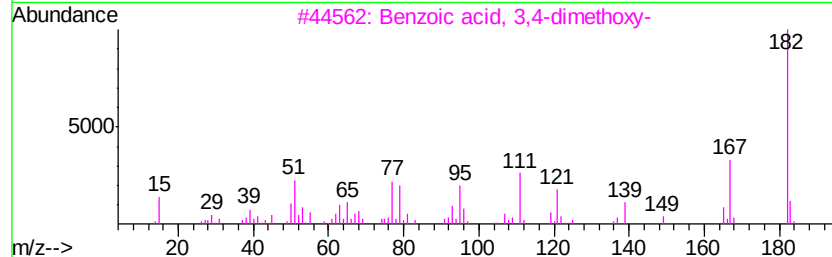
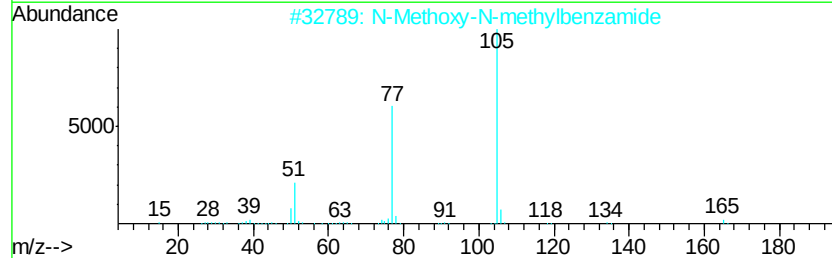
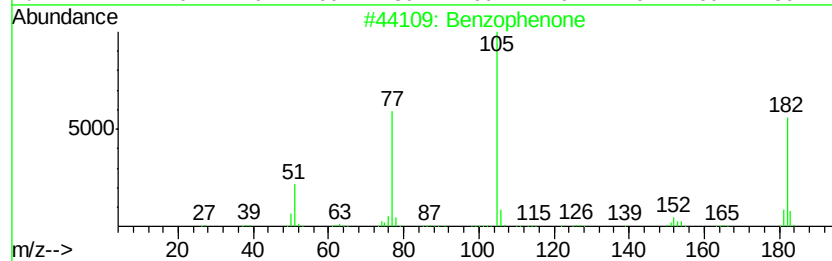
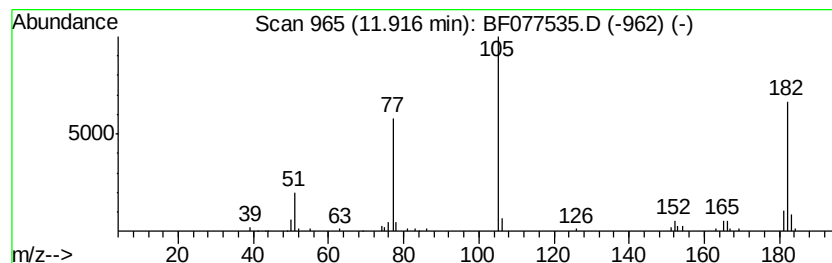
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.49 ng	105796	Acenaphthene-d10	11.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 95
2		N-Methoxy-N-methylbenzamide	165 C9H11NO2	006919-61-5 46
3		Benzoic acid, 3,4-dimethoxy-	182 C9H10O4	000093-07-2 43
4		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 43
5		Benzoic acid, phenyl ester	198 C13H10O2	000093-99-2 38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030215\
Data File : BF077535.D
Acq On : 2 Mar 2015 21:18
Operator : TP/IZ
Sample : G1399-09
Misc : S
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB3

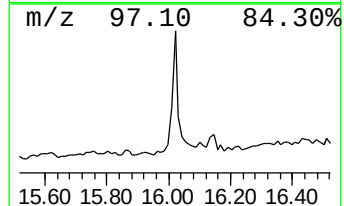
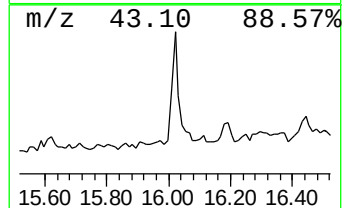
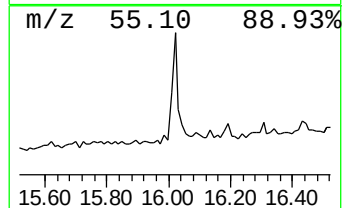
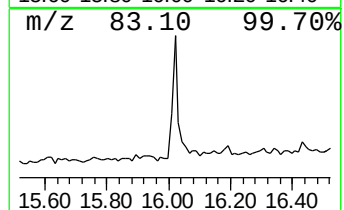
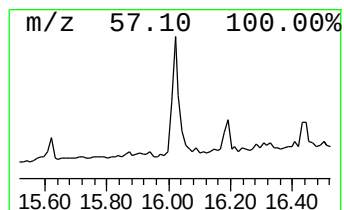
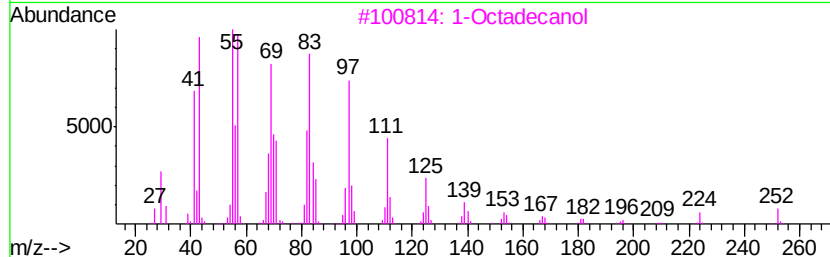
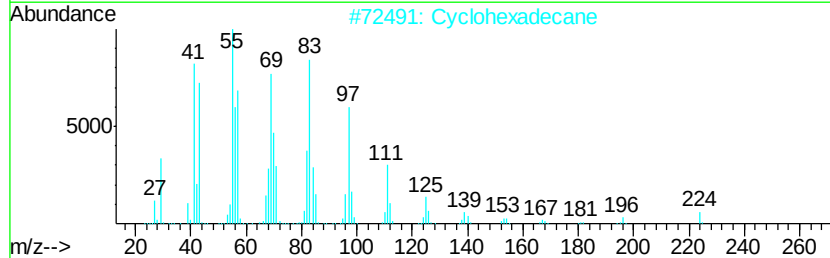
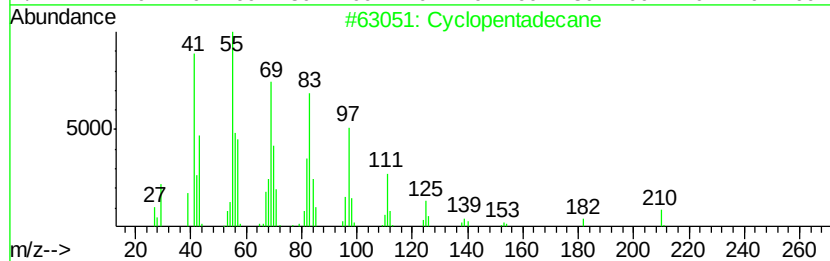
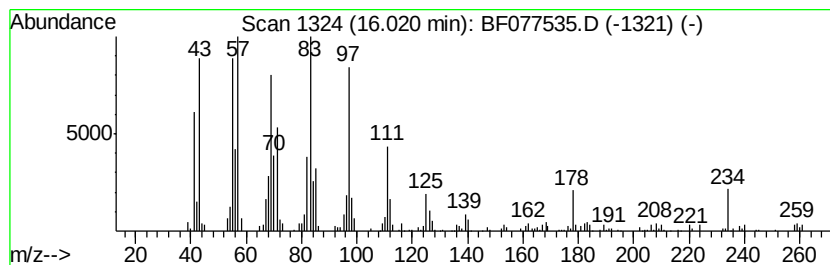
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclopentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.92 ng	226426	Chrysene-d12	16.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	98
2		Cyclohexadecane	224	C16H32	000295-65-8	97
3		1-Octadecanol	270	C18H38O	000112-92-5	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		1-Nonadecene	266	C19H38	018435-45-5	87



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Sample : G1399-09
Misc : S
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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
Cyclopentane, met...	1.18	51.0	ng	1324230	1	7.26	518765	20.0
Propane, 2,2-dime...	1.41	205.2	ng	5322160	1	7.26	518765	20.0
Butane, 2-methoxy...	1.72	12.3	ng	319508	1	7.26	518765	20.0
2-Pentanone, 4-hy...	5.04	12.5	ng	325376	1	7.26	518765	20.0
unknown6.97	6.97	61.9	ng	1606010	1	7.26	518765	20.0
Benzophenone	11.92	2.5	ng	105796	3	11.01	848635	20.0
Cyclopentadecane	16.02	2.9	ng	226426	5	16.15	1552300	20.0