

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
 Data File : BF099474.D
 Acq On : 14 Oct 2017 13:59
 Operator : SJ/JU
 Sample : I5819-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 4098-QC-1

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-BF092317.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	2.275	29	32	38	rVB	255599	210998	6.05%	0.606%
2	3.957	313	318	326	rBV	76179	105514	3.03%	0.303%
3	5.081	506	509	525	rVB	289786	377790	10.84%	1.084%
4	5.487	574	578	597	rVB	1751687	1695793	48.66%	4.867%
5	6.487	744	748	768	rBV	1264406	1101400	31.60%	3.161%
6	6.628	768	772	775	rBV	2804490	2577224	73.95%	7.397%
7	6.851	807	810	817	rVB	690153	566886	16.27%	1.627%
8	7.010	833	837	840	rBV	2624021	2378377	68.24%	6.826%
9	7.422	902	907	910	rBV	1887118	1875320	53.81%	5.382%
10	8.134	1024	1028	1030	rBV	927186	827782	23.75%	2.376%
11	8.157	1030	1032	1046	rVB	770785	619147	17.77%	1.777%
12	8.845	1145	1149	1153	rBV	1156949	1006764	28.89%	2.889%
13	8.945	1162	1166	1170	rBV	946979	769180	22.07%	2.208%
14	9.210	1206	1211	1214	rBV	3502618	3485191	100.00%	10.003%
15	9.751	1299	1303	1313	rBV	671129	546050	15.67%	1.567%
16	9.886	1323	1326	1329	rBV	938151	831915	23.87%	2.388%
17	9.922	1329	1332	1335	rVB	615339	496917	14.26%	1.426%
18	10.439	1416	1420	1423	rBV	1659021	1373208	39.40%	3.941%
19	10.680	1457	1461	1465	rBV	1682486	1788422	51.31%	5.133%
20	11.380	1576	1580	1581	rBV	862881	788146	22.61%	2.262%
21	11.410	1581	1585	1588	rVV	2747796	2697286	77.39%	7.741%
22	11.457	1588	1593	1598	rVB	524257	494299	14.18%	1.419%
23	12.592	1782	1786	1790	rBV	1755329	1679995	48.20%	4.822%
24	12.821	1818	1825	1829	rBV	755450	661872	18.99%	1.900%
25	12.963	1844	1849	1852	rBV	2814035	2849283	81.75%	8.178%
26	14.016	2023	2028	2031	rBV2	609831	777791	22.32%	2.232%
27	14.045	2031	2033	2044	rVB	903912	753887	21.63%	2.164%
28	15.057	2202	2205	2208	rBV	226825	265809	7.63%	0.763%
29	15.086	2208	2210	2221	rVB	210838	238147	6.83%	0.684%
30	15.433	2264	2269	2274	rBV	81999	107718	3.09%	0.309%
31	15.492	2274	2279	2288	rVB	320284	409174	11.74%	1.174%
32	16.980	2525	2532	2547	rBV3	168560	387748	11.13%	1.113%
33	17.433	2603	2609	2620	rBV2	38506	97148	2.79%	0.279%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

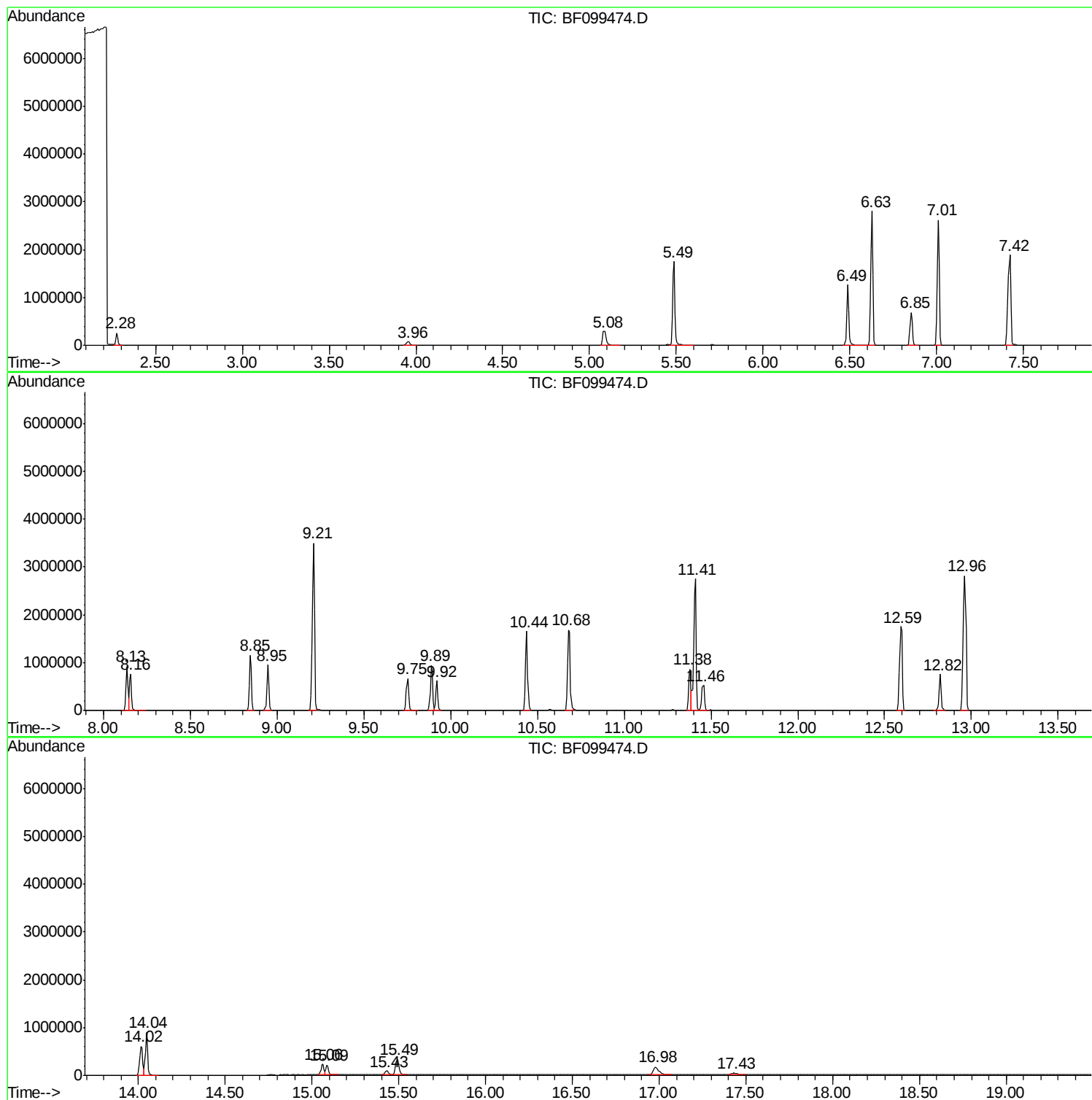
Sum of corrected areas: 34842181

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

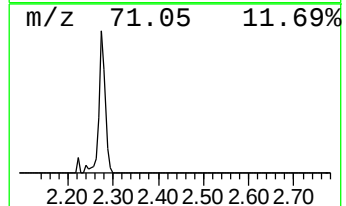
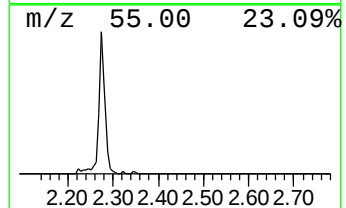
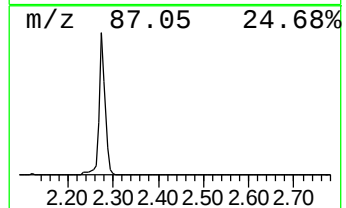
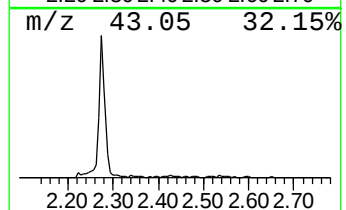
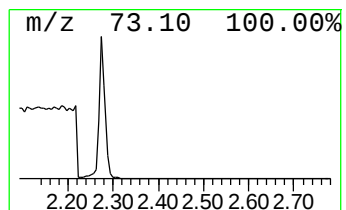
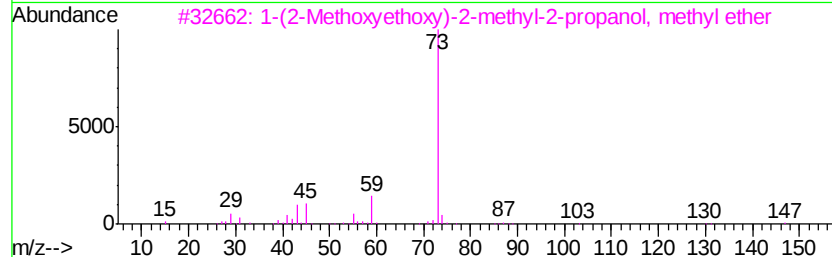
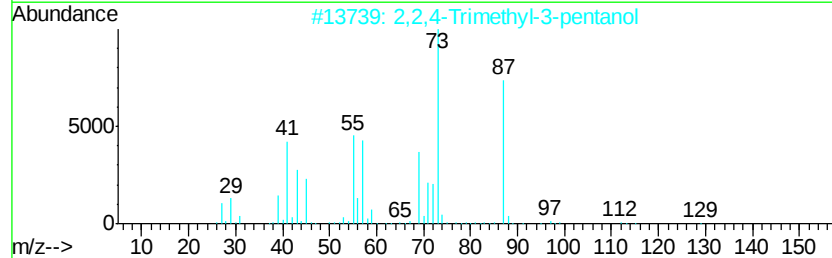
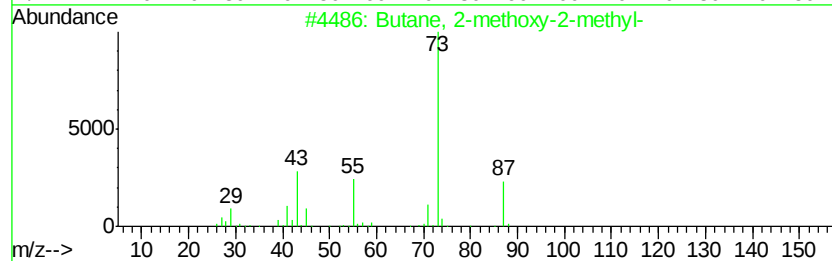
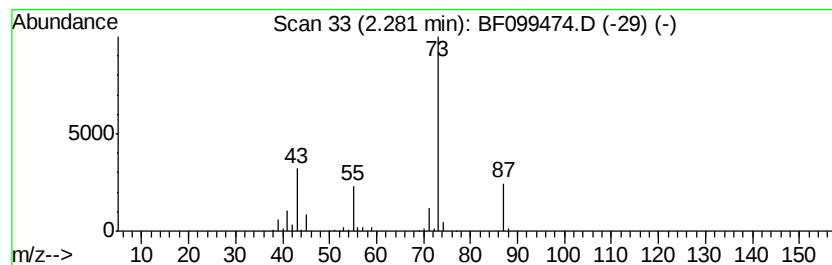
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	7.44 ng	210998	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

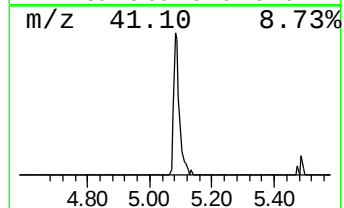
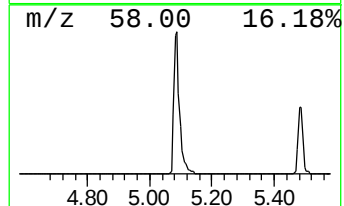
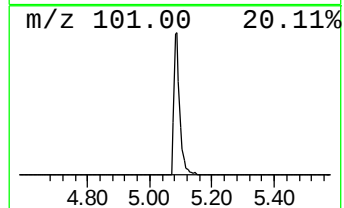
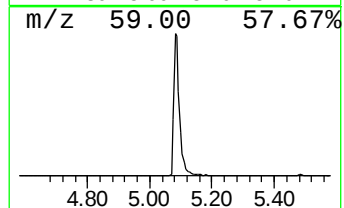
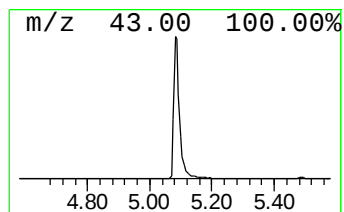
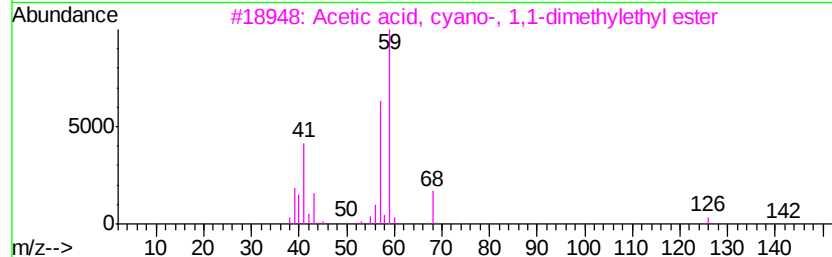
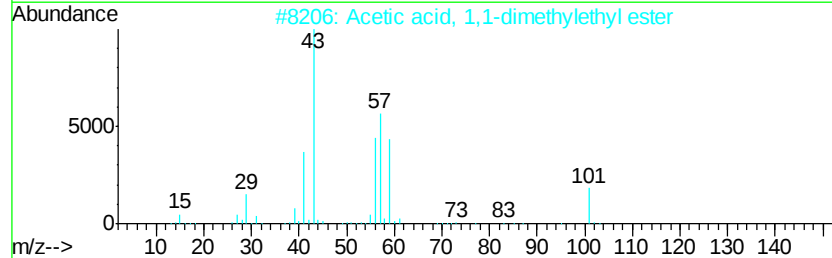
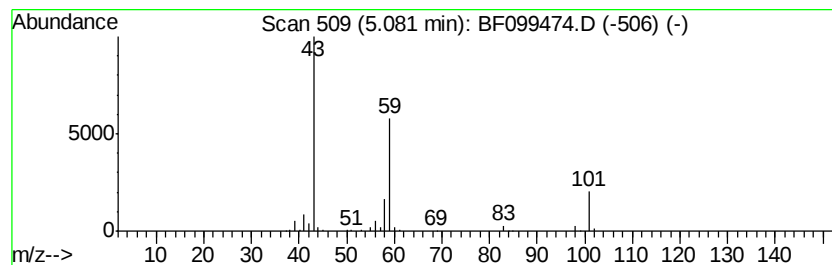
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	13.33 ng	377790	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

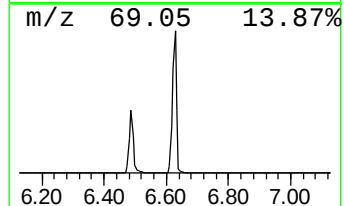
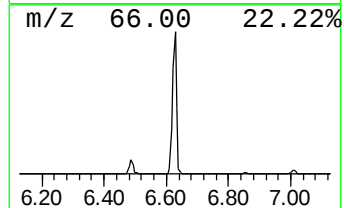
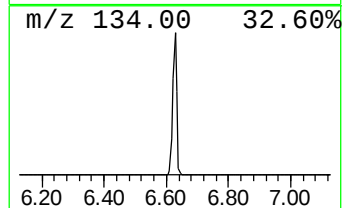
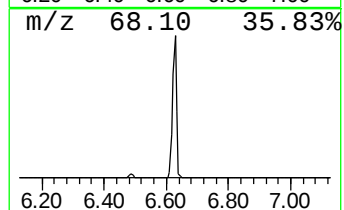
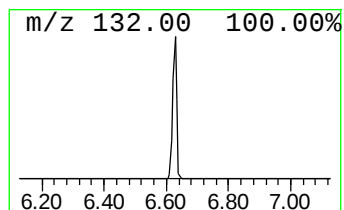
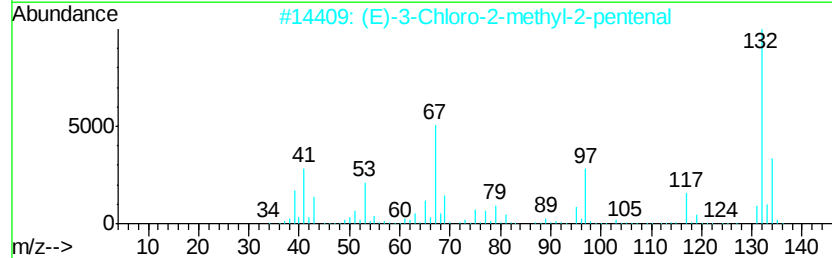
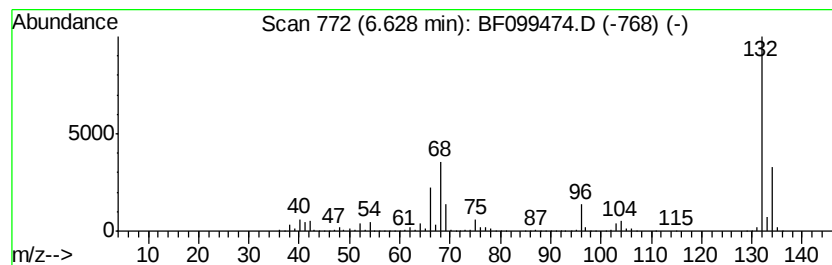
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	90.93 ng	2577220	1,4-Dichlorobenzene-d4	6.85

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

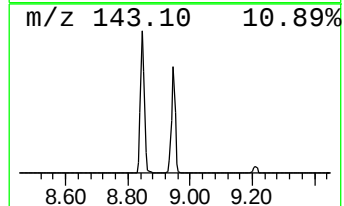
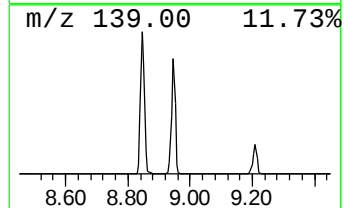
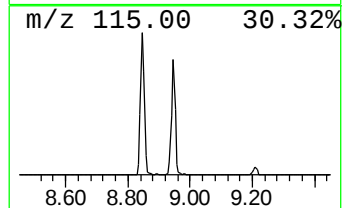
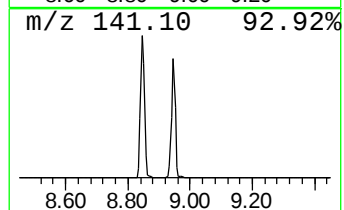
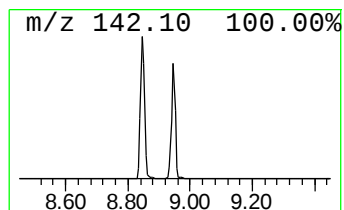
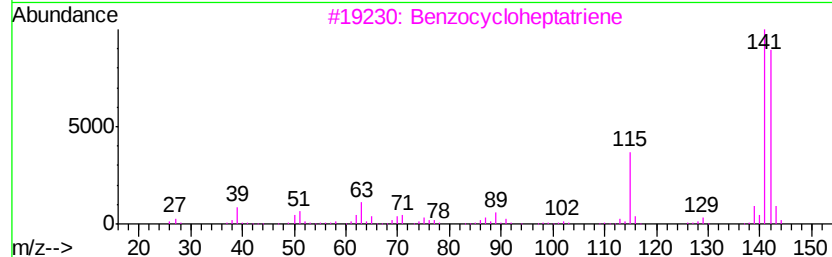
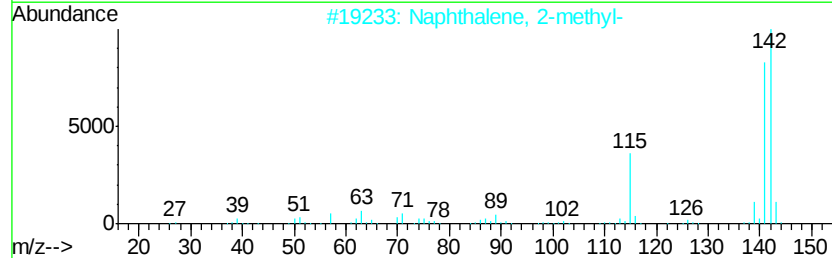
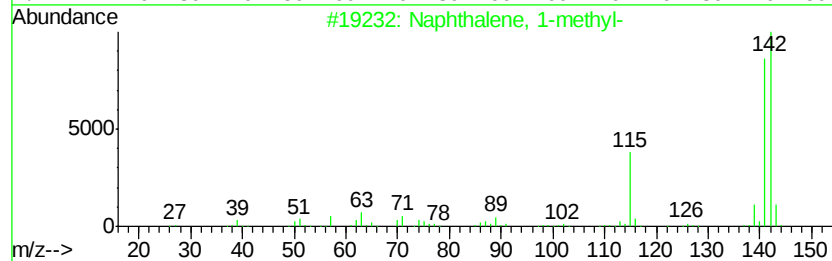
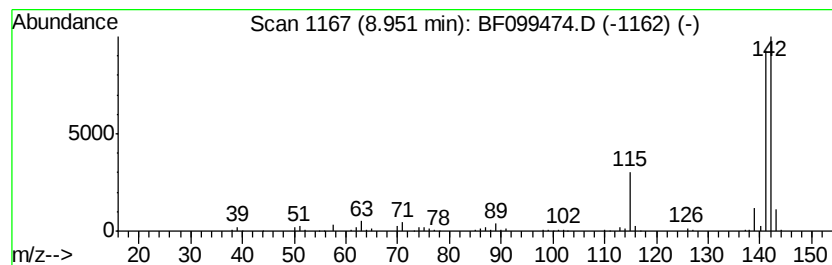
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	18.58 ng	769180	Naphthalene-d8	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	91
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099474.D
Acq On : 14 Oct 2017 13:59
Operator : SJ/JU
Sample : I5819-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4098-QC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.28	7.4	ng	210998	1	6.85	566886	20.0
2-Pentanone, 4-hy...	5.08	13.3	ng	377790	1	6.85	566886	20.0
unknown6.63	6.63	90.9	ng	2577220	1	6.85	566886	20.0
Naphthalene, 1-me...	8.95	18.6	ng	769180	2	8.13	827782	20.0