

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
 Data File : BF102864.D
 Acq On : 8 Feb 2018 18:55
 Operator : SJ/JU
 Sample : J1470-13
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-11

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-BF020318.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	2.157	7	12	21	rVB	405130	512368	11.73%	1.255%
2	5.116	512	515	525	rVB	120362	149851	3.43%	0.367%
3	5.504	576	581	584	rBV	4342283	4262672	97.56%	10.438%
4	6.516	747	753	768	rBV	3823410	4369089	100.00%	10.699%
5	6.657	772	777	780	rBV	4285086	4142929	94.82%	10.145%
6	6.887	812	816	819	rBV	1464855	1201358	27.50%	2.942%
7	7.039	838	842	846	rBV	3072538	2912426	66.66%	7.132%
8	7.445	906	911	914	rBV	2663485	2682796	61.40%	6.570%
9	7.522	921	924	930	rVB2	48387	45883	1.05%	0.112%
10	8.169	1030	1034	1037	rBV	1791655	1467501	33.59%	3.594%
11	9.239	1212	1216	1220	rBV	3491885	3272963	74.91%	8.015%
12	9.316	1226	1229	1232	rVB	93963	68855	1.58%	0.169%
13	9.633	1279	1283	1286	rBV	396838	339491	7.77%	0.831%
14	9.845	1312	1319	1322	rBV	211707	188456	4.31%	0.461%
15	9.922	1329	1332	1336	rBV	1383698	1293888	29.61%	3.168%
16	10.169	1370	1374	1378	rBV2	41999	44459	1.02%	0.109%
17	10.322	1397	1400	1402	rBV	59035	52013	1.19%	0.127%
18	10.345	1402	1404	1407	rVB	212286	154327	3.53%	0.378%
19	10.563	1437	1441	1444	rBV	48271	66700	1.53%	0.163%
20	10.669	1457	1459	1461	rBV	106232	91982	2.11%	0.225%
21	10.710	1463	1466	1476	rVB	1683058	1687458	38.62%	4.132%
22	10.816	1482	1484	1486	rBV	223703	232486	5.32%	0.569%
23	10.833	1486	1487	1490	rVV	355708	281792	6.45%	0.690%
24	10.886	1493	1496	1499	rBV	770710	696818	15.95%	1.706%
25	10.922	1499	1502	1505	rVV2	630792	784785	17.96%	1.922%
26	10.957	1505	1508	1510	rVV	719929	626472	14.34%	1.534%
27	10.980	1510	1512	1514	rVV	450691	341153	7.81%	0.835%
28	11.022	1514	1519	1520	rVV2	302346	355779	8.14%	0.871%
29	11.033	1520	1521	1524	rVV	250100	221773	5.08%	0.543%
30	11.069	1524	1527	1530	rVV3	622911	688280	15.75%	1.685%
31	11.104	1530	1533	1535	rVV	737822	619764	14.19%	1.518%
32	11.127	1535	1537	1538	rVV	187102	165948	3.80%	0.406%
33	11.145	1538	1540	1545	rVB2	424861	352640	8.07%	0.864%
34	11.227	1550	1554	1558	rBV	40249	52916	1.21%	0.130%

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ClientSampleId :
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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	11.269	1558	1561	1563	rBV	102703	87097	1.99%	0.213%
36	11.292	1563	1565	1568	rVB2	61614	52512	1.20%	0.129%
37	11.416	1582	1586	1589	rBV	1059796	997259	22.83%	2.442%
38	12.810	1820	1823	1826	rBV	69624	55484	1.27%	0.136%
39	12.874	1830	1834	1843	rVB	436911	457161	10.46%	1.119%
40	12.998	1850	1855	1858	rBV	2375398	2194078	50.22%	5.373%
41	13.468	1932	1935	1939	rBV	43358	46565	1.07%	0.114%
42	13.880	2002	2005	2012	rBV	302457	304187	6.96%	0.745%
43	14.021	2026	2029	2031	rBV	84785	78405	1.79%	0.192%
44	14.051	2031	2034	2040	rVB	993334	1006974	23.05%	2.466%
45	14.492	2107	2109	2111	rBV	54567	56540	1.29%	0.138%
46	15.162	2220	2223	2226	rBV	72819	82582	1.89%	0.202%
47	15.539	2282	2287	2294	rBV	638319	889997	20.37%	2.179%
48	15.998	2362	2365	2369	rVB2	74616	99331	2.27%	0.243%

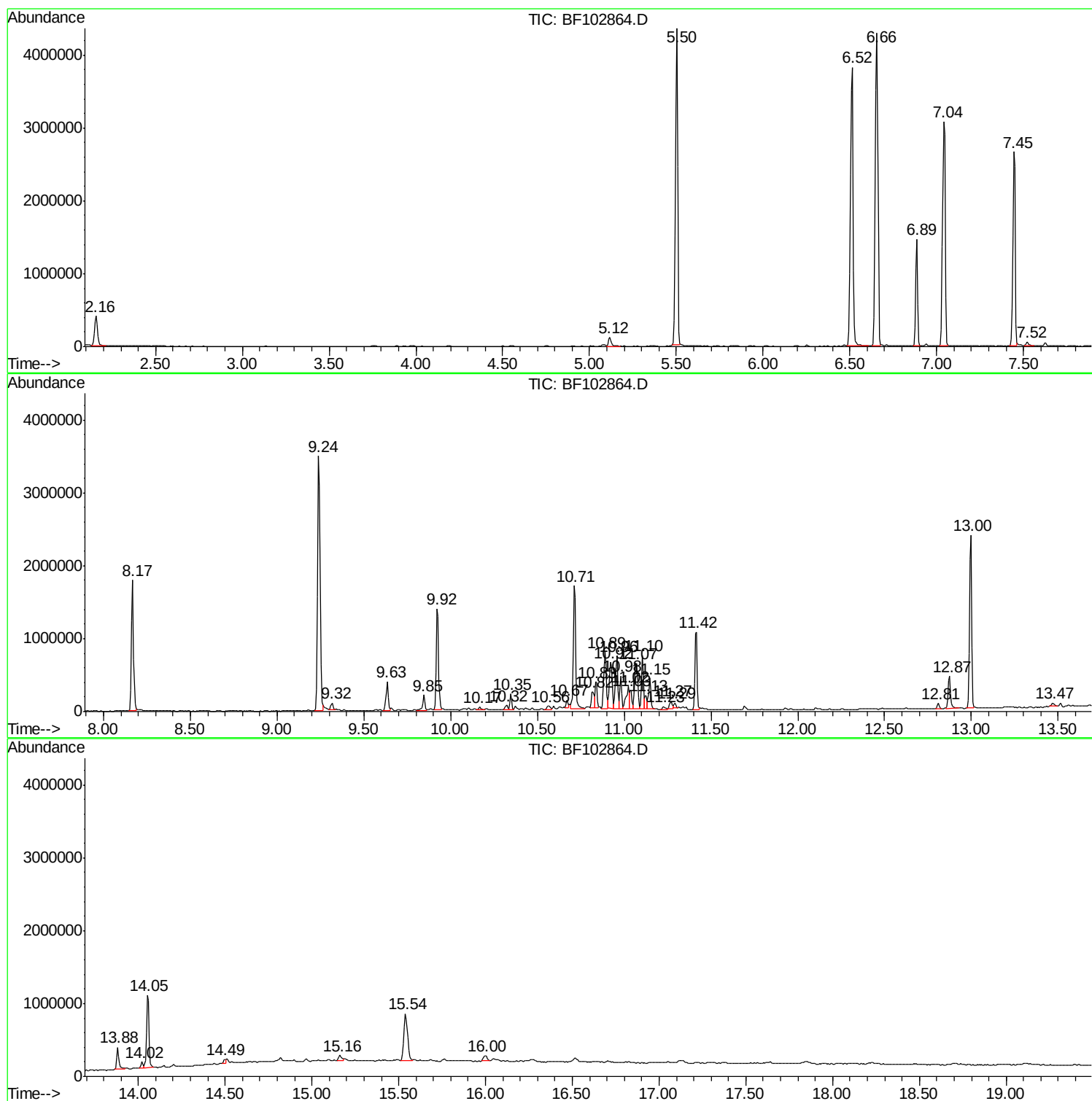
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BNA_F
ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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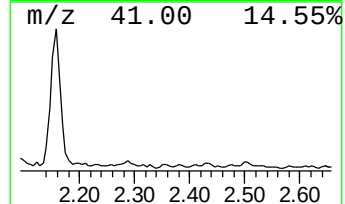
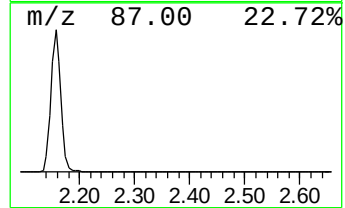
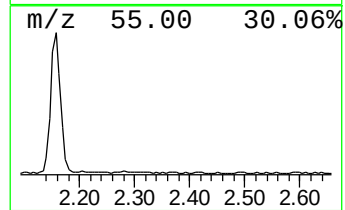
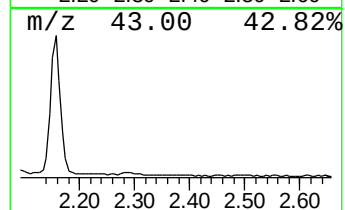
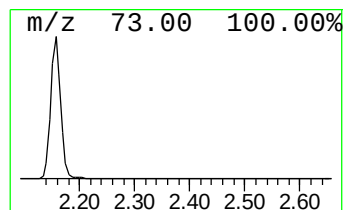
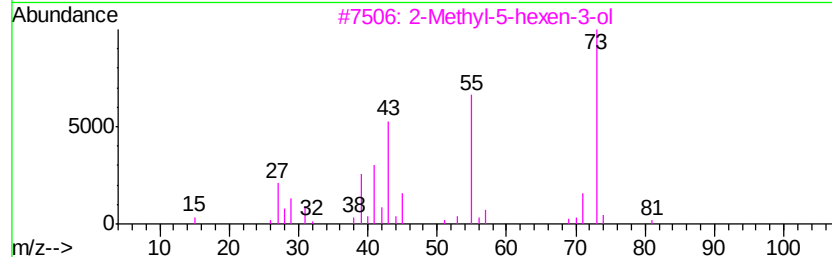
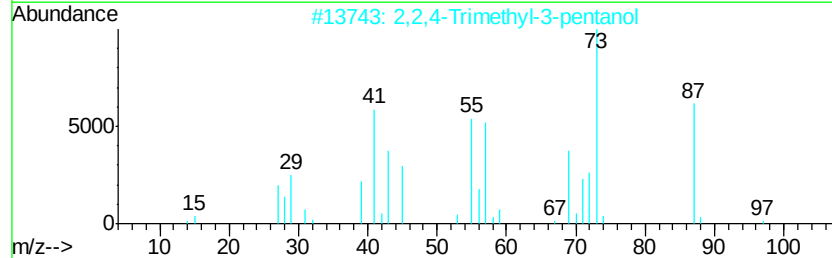
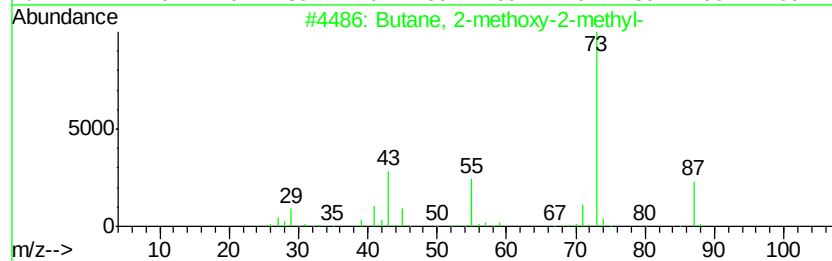
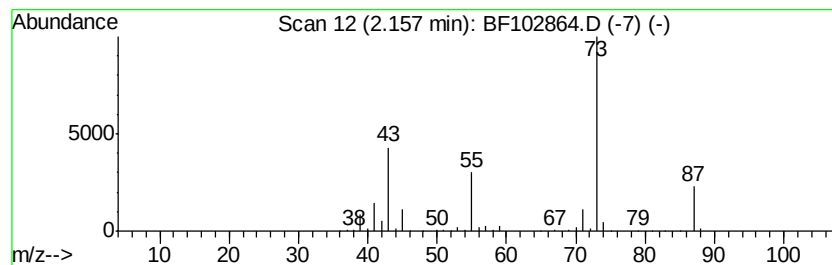
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	8.53 ng	512368	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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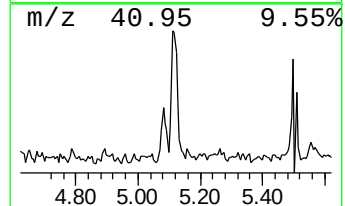
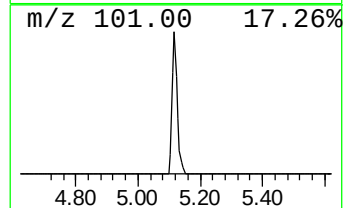
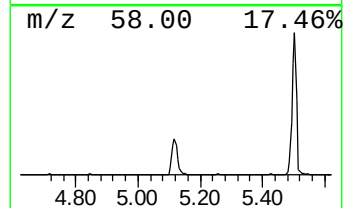
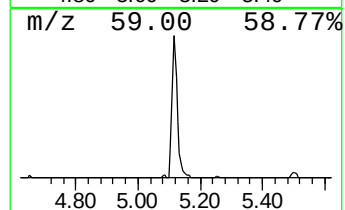
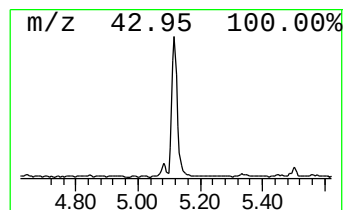
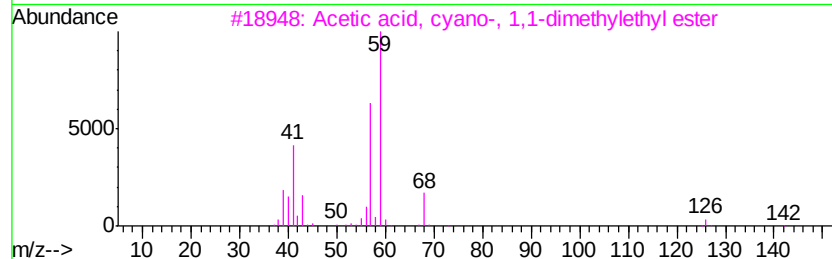
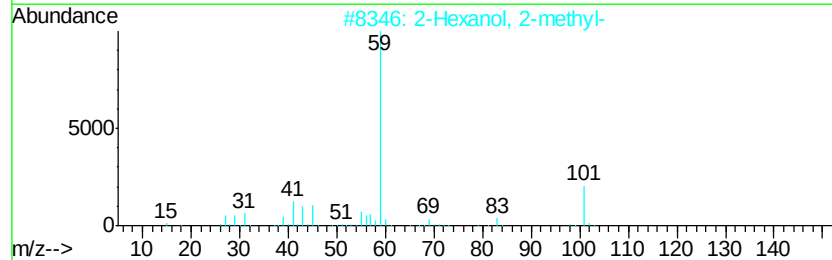
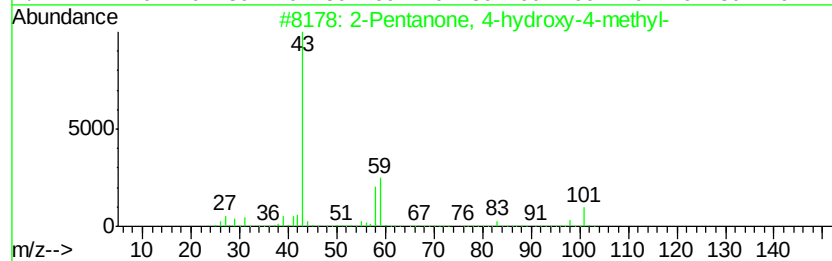
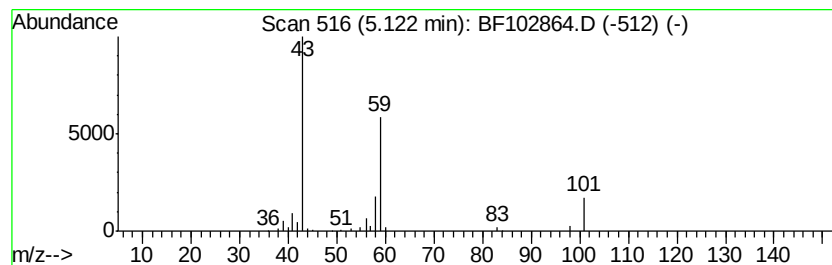
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.49 ng	149851	1,4-Dichlorobenzene-d4	6.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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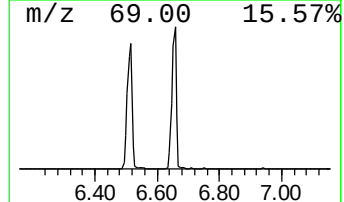
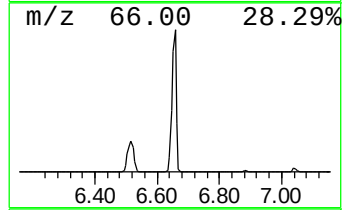
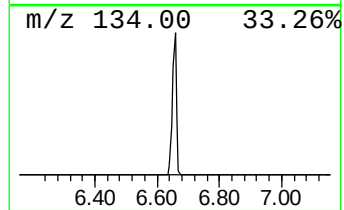
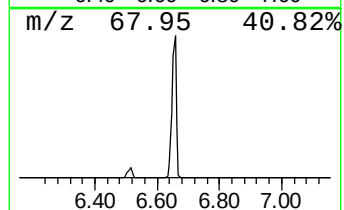
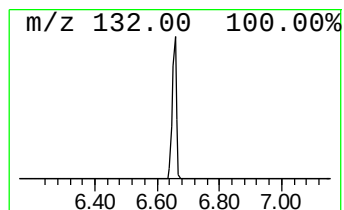
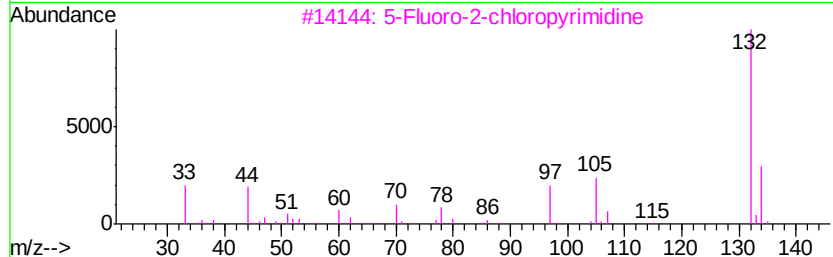
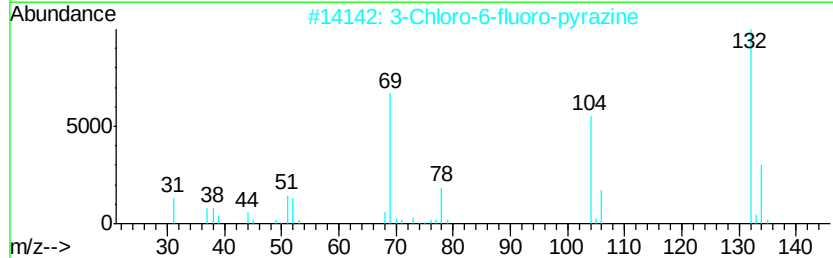
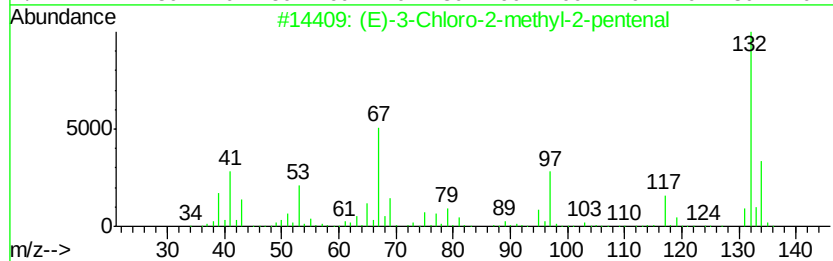
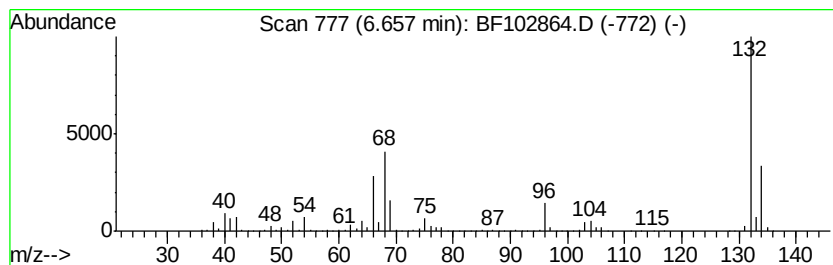
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.97 ng	4142930	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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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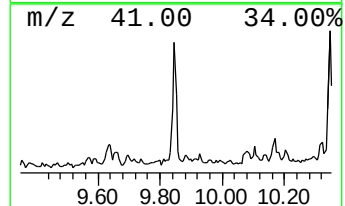
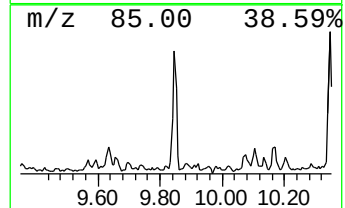
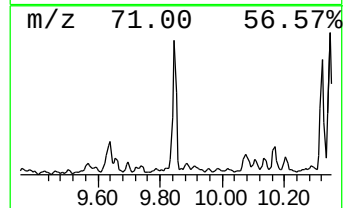
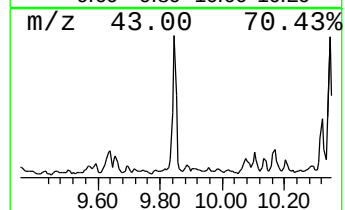
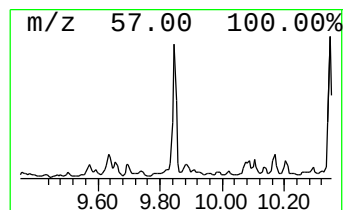
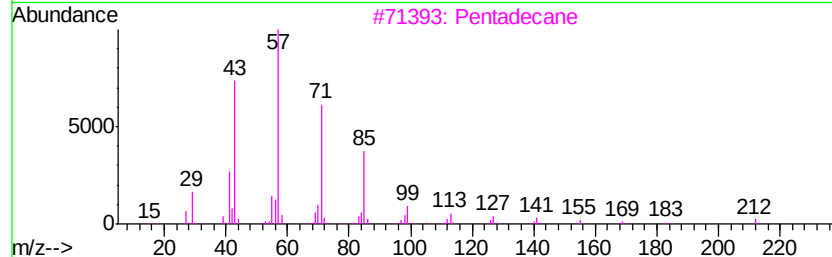
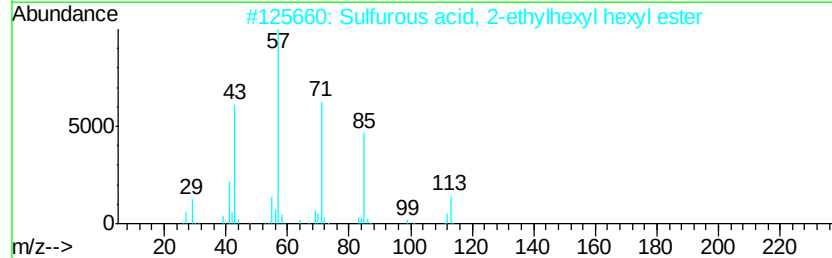
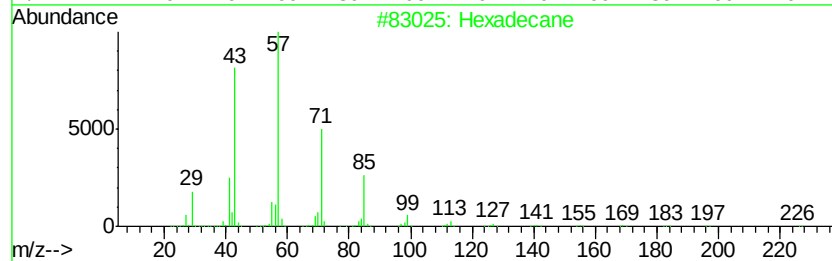
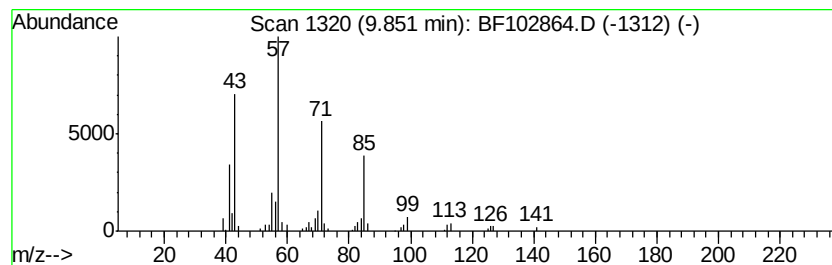
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.91 ng	188456	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	87
2	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	86
3	Pentadecane	212 C15H32	000629-62-9	86
4	Nonane, 5-butyl-	184 C13H28	017312-63-9	64
5	Decane, 3-bromo-	220 C10H21Br	030571-71-2	59



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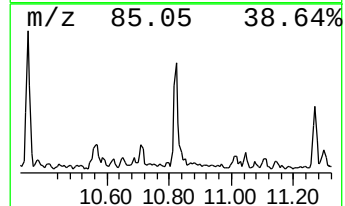
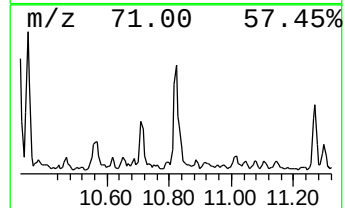
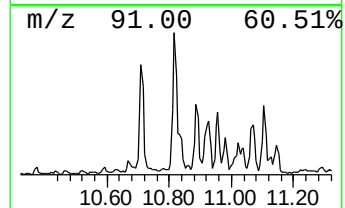
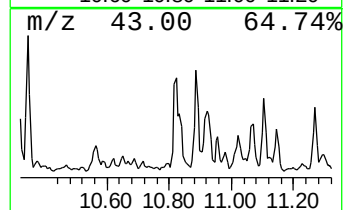
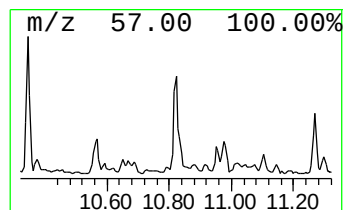
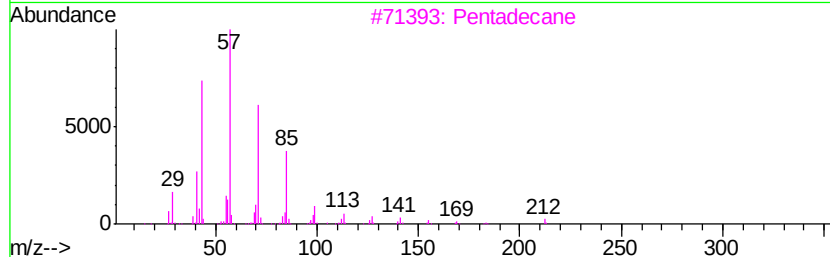
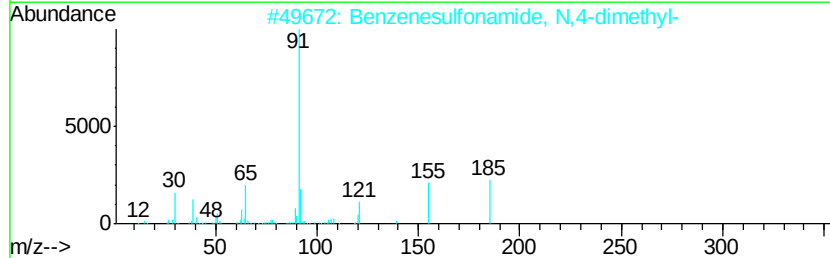
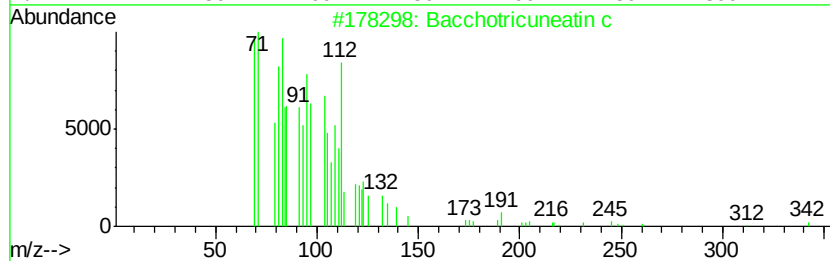
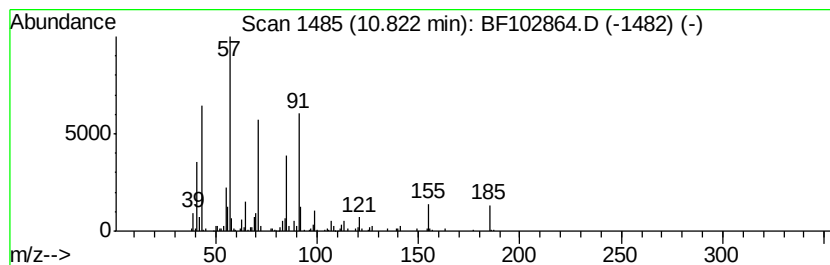
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3N-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bacchotricuneatin c Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	4.66 ng	232486	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	94
2	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	80
3	Pentadecane	212	C15H32	000629-62-9	45
4	Hexadecane	226	C16H34	000544-76-3	45
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102864.D
Acq On : 8 Feb 2018 18:55
Operator : SJ/JU
Sample : J1470-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.83 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	5.65 ng	281792	Phenanthrene-d10	11.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	43
2			2-Acetamidotropone	163	C9H9NO2	006422-12-4	38
3			Benzenemethanol, 4-methyl-.alpha...	176	C12H16O	083173-76-6	38
4			Silane, trimethoxypropyl-	164	C6H16O3Si	001067-25-0	32
5			Carbonic acid, ethyl 4-isopropyl...	208	C12H16O3	1000331-34-2	32

