

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072518\
 Data File : BF107668.D
 Acq On : 25 Jul 2018 20:17
 Operator : JU/SJ
 Sample : J4031-03 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PLANTER-DOC-3

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	5.196	482	486	497	rBV	305506	338692	15.33%	1.284%
2	5.596	550	554	581	rBV	1414948	1994057	90.26%	7.557%
3	6.595	721	724	744	rBV	1350815	2055081	93.02%	7.788%
4	6.737	744	748	764	rVV	1883860	2141478	96.94%	8.116%
5	6.966	784	787	810	rBV	946858	1131724	51.23%	4.289%
6	7.119	810	813	830	rBV	1478482	1675085	75.82%	6.348%
7	7.531	879	883	902	rBV	906894	1266780	57.34%	4.801%
8	8.248	1001	1005	1026	rBV	1287703	1457717	65.98%	5.524%
9	9.319	1184	1187	1197	rBV	2105069	2209189	100.00%	8.372%
10	9.425	1203	1205	1214	rVB5	16137	24631	1.11%	0.093%
11	9.713	1251	1254	1260	rBV	148156	139095	6.30%	0.527%
12	9.872	1278	1281	1286	rVB	38886	40921	1.85%	0.155%
13	10.007	1301	1304	1309	rBV2	1323320	1314527	59.50%	4.982%
14	10.413	1368	1373	1378	rBV2	48714	54862	2.48%	0.208%
15	10.560	1395	1398	1401	rBV2	24794	23666	1.07%	0.090%
16	10.801	1435	1439	1452	rBV	1128078	1245219	56.37%	4.719%
17	10.913	1452	1458	1466	rVB3	58717	127885	5.79%	0.485%
18	11.342	1528	1531	1533	rBV3	27094	24792	1.12%	0.094%
19	11.507	1555	1559	1561	rBV	1085185	1172177	53.06%	4.442%
20	11.530	1561	1563	1569	rVV	347867	360463	16.32%	1.366%
21	11.583	1569	1572	1575	rVB	62746	70512	3.19%	0.267%
22	11.742	1594	1599	1602	rBV2	20107	36621	1.66%	0.139%
23	12.007	1641	1644	1646	rBV	104204	99051	4.48%	0.375%
24	12.036	1646	1649	1653	rVB2	54214	61953	2.80%	0.235%
25	12.119	1660	1663	1665	rBV	84601	81478	3.69%	0.309%
26	12.301	1691	1694	1696	rBV	33791	35719	1.62%	0.135%
27	12.330	1696	1699	1705	rVB5	40888	62382	2.82%	0.236%
28	12.554	1735	1737	1739	rBV2	28514	27907	1.26%	0.106%
29	12.724	1762	1766	1771	rBV	666087	692944	31.37%	2.626%
30	12.936	1799	1802	1803	rBV2	136402	143949	6.52%	0.546%
31	12.954	1803	1805	1811	rVB	636860	561381	25.41%	2.127%
32	13.089	1824	1828	1835	rBV	1667483	1737836	78.66%	6.586%
33	13.513	1898	1900	1903	rBV	125372	112033	5.07%	0.425%
34	13.971	1975	1978	1981	rVB3	133999	122540	5.55%	0.464%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.154	2004	2009	2012	rBV2	1213825	1552908	70.29%	5.885%
36	14.183	2012	2014	2022	rVB	383013	394634	17.86%	1.496%
37	15.230	2189	2192	2195	rBV	234729	339446	15.37%	1.286%
38	15.624	2256	2259	2264	rBV	184704	288507	13.06%	1.093%
39	15.695	2266	2271	2279	rVV	675359	1167099	52.83%	4.423%

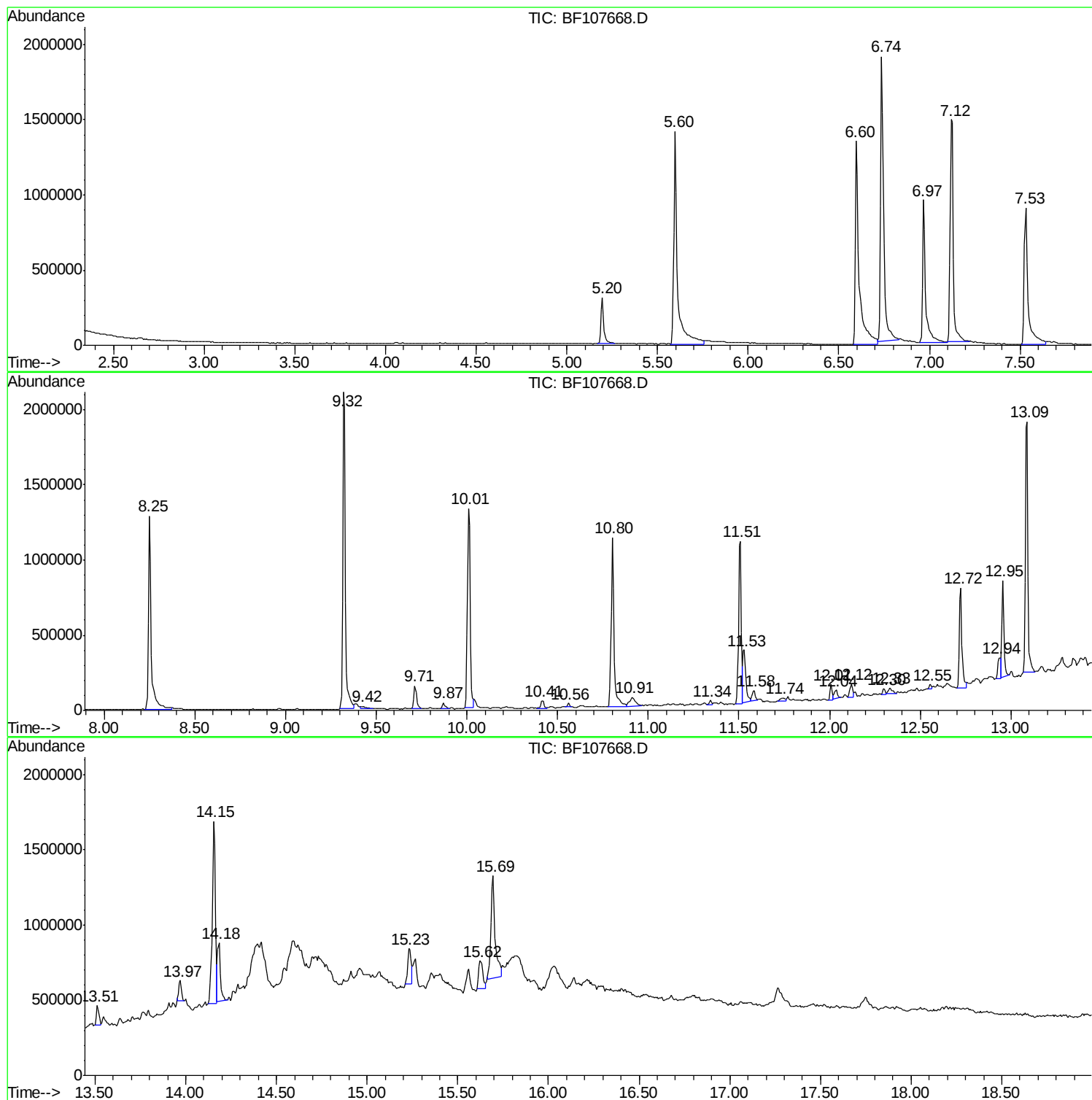
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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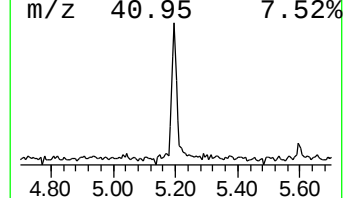
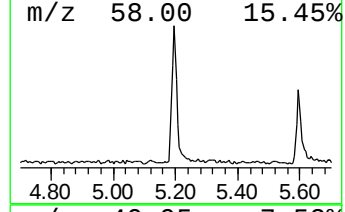
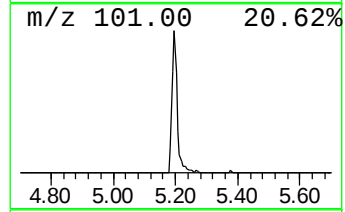
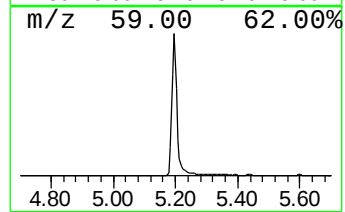
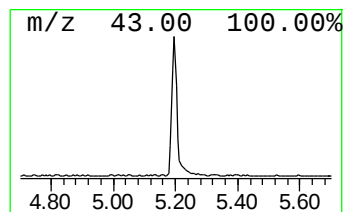
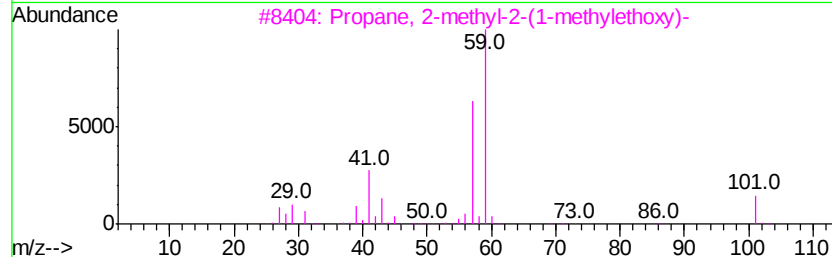
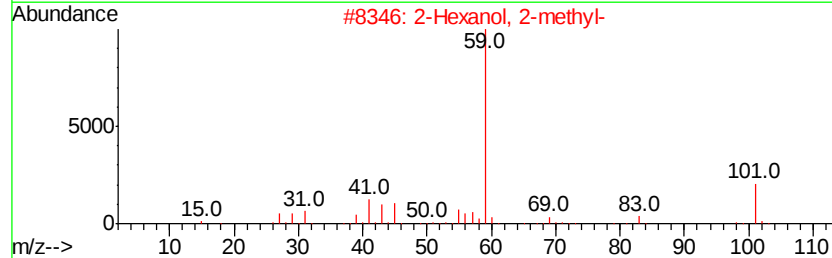
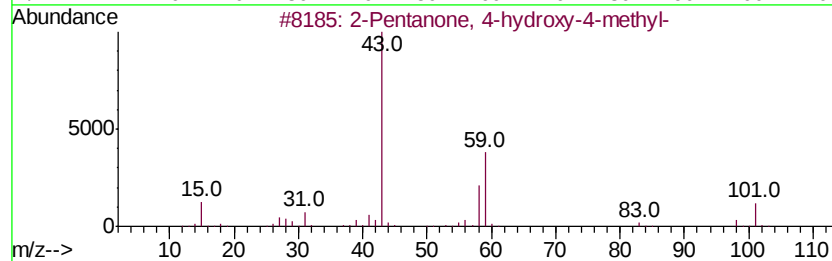
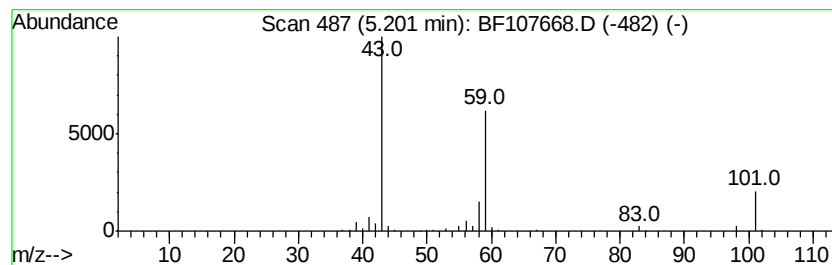
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.20	5.99 ng	338692	1,4-Dichlorobenzene-d4	6.97

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	38
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25



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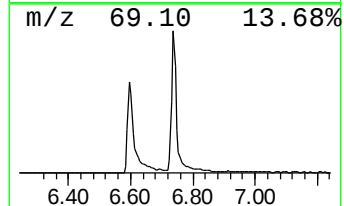
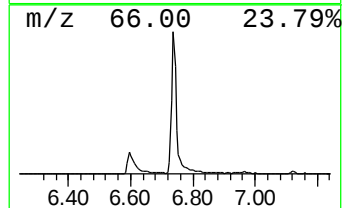
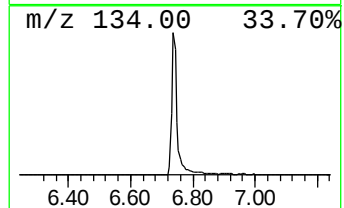
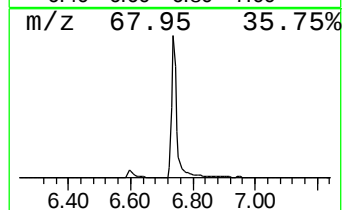
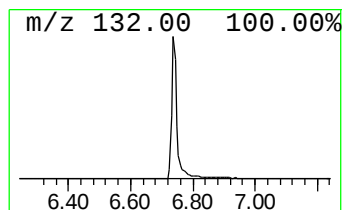
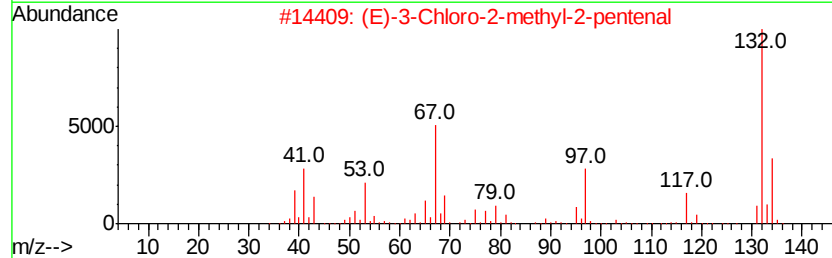
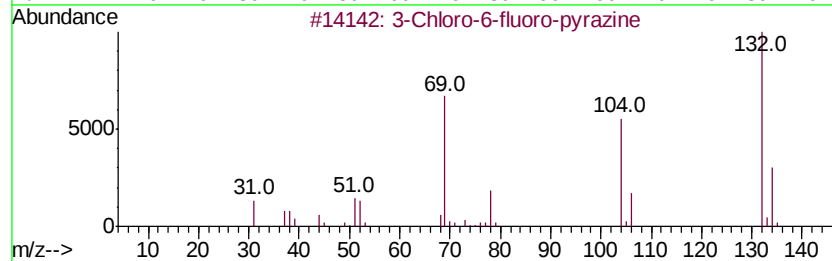
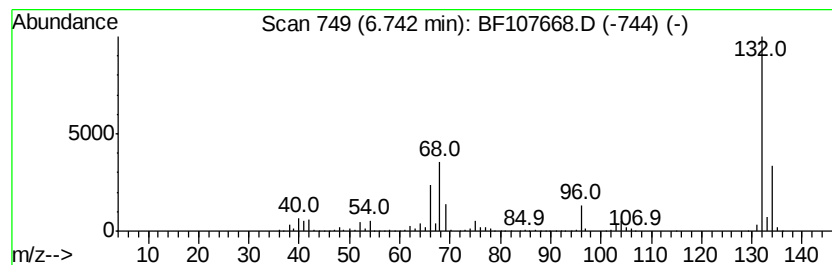
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	37.84 ng	2141480	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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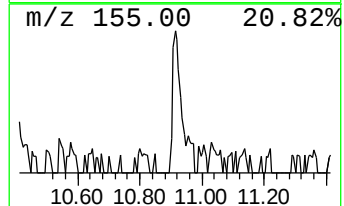
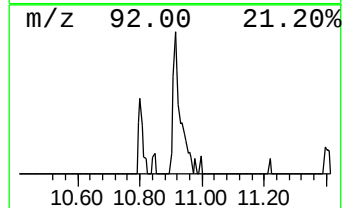
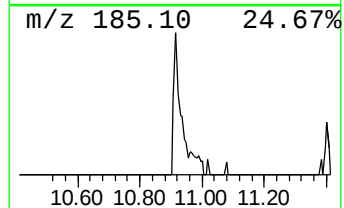
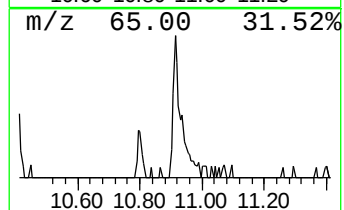
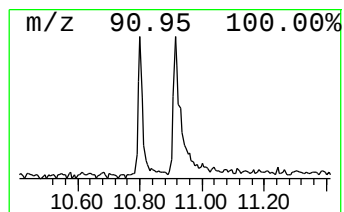
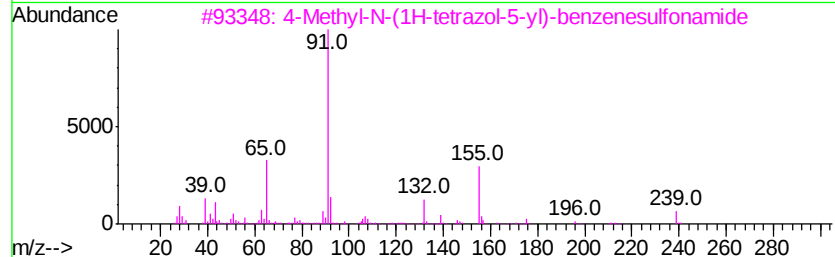
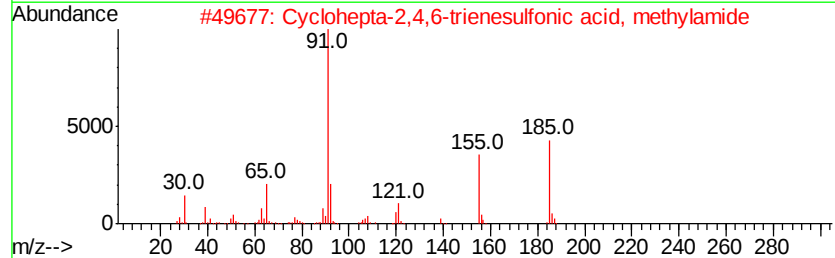
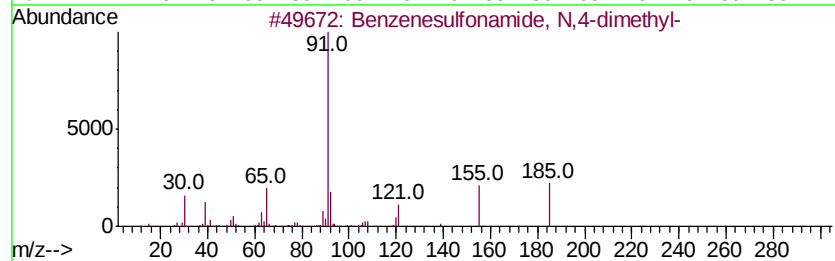
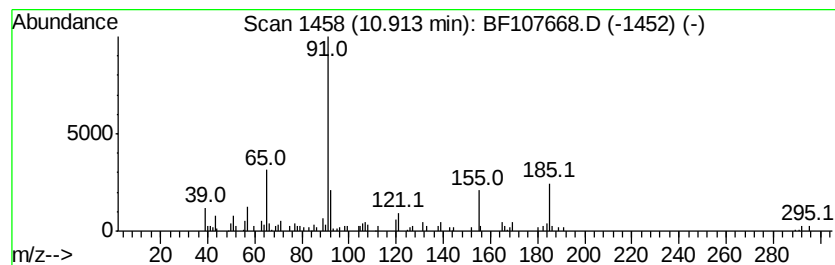
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.18 ng	127885	Phenanthrene-d10	11.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	81
2		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3		4-Methyl-N-(1H-tetrazol-5-yl)-be...	239	C8H9N5O2S	006455-80-7	43
4		Benzenesulfonic acid, 4-methyl-,...	292	C15H21BO3S	1000153-16-3	43
5		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	38



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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...	5.20	6.0	ng	338692	1	6.97	1131720	20.0
unknown6.74	6.74	37.8	ng	2141480	1	6.97	1131720	20.0
Benzenesulfonamid...	10.91	2.2	ng	127885	4	11.51	1172180	20.0