

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
 Data File : BF108816.D
 Acq On : 6 Sep 2018 10:45
 Operator : JU/SJ
 Sample : J4741-02
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AOC2-03-B

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-BF090518.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	3.313	157	166	175	rVB2	19437	36284	1.96%	0.204%
2	4.278	325	330	337	rBV	1534506	1853203	100.00%	10.399%
3	4.919	434	439	445	rBV	1264239	1401060	75.60%	7.862%
4	5.331	506	509	514	rVB	104105	93603	5.05%	0.525%
5	6.354	680	683	690	rBV	505755	406383	21.93%	2.280%
6	6.495	704	707	711	rBV	244637	202508	10.93%	1.136%
7	6.736	744	748	751	rBV	1733403	1412930	76.24%	7.928%
8	6.889	770	774	778	rBV	1031311	807193	43.56%	4.529%
9	7.054	799	802	806	rVB	24102	20237	1.09%	0.114%
10	7.289	838	842	845	rBV	719876	576231	31.09%	3.233%
11	8.019	962	966	969	rBV	1969831	1739863	93.88%	9.763%
12	8.042	969	970	977	rVB3	35374	35524	1.92%	0.199%
13	9.089	1144	1148	1151	rBV	1533918	1121881	60.54%	6.295%
14	9.436	1203	1207	1209	rBV3	21351	21479	1.16%	0.121%
15	9.483	1211	1215	1218	rBV	363553	271567	14.65%	1.524%
16	9.766	1259	1263	1267	rBV	1992602	1656013	89.36%	9.292%
17	10.107	1317	1321	1325	rBV3	22619	21761	1.17%	0.122%
18	10.689	1416	1420	1424	rBV3	21853	29851	1.61%	0.168%
19	10.742	1426	1429	1431	rBV2	36809	35585	1.92%	0.200%
20	10.772	1431	1434	1437	rVB3	27421	29547	1.59%	0.166%
21	10.830	1442	1444	1446	rBV	43874	31650	1.71%	0.178%
22	10.919	1456	1459	1462	rBV2	39133	34870	1.88%	0.196%
23	11.130	1490	1495	1498	rBV3	15598	20309	1.10%	0.114%
24	11.207	1505	1508	1510	rBV	21459	20709	1.12%	0.116%
25	11.242	1510	1514	1517	rVV	1737357	1414292	76.32%	7.936%
26	11.266	1517	1518	1521	rVV	74178	35592	1.92%	0.200%
27	11.313	1524	1526	1531	rVB	30242	26335	1.42%	0.148%
28	12.024	1644	1647	1650	rBV3	18418	20771	1.12%	0.117%
29	12.448	1716	1719	1722	rVB	95345	88961	4.80%	0.499%
30	12.671	1752	1757	1760	rBV	92668	105259	5.68%	0.591%
31	12.718	1763	1765	1772	rVB8	21957	31105	1.68%	0.175%
32	12.818	1779	1782	1786	rBV	1037908	918735	49.58%	5.155%
33	13.071	1822	1825	1827	rBV3	26483	24055	1.30%	0.135%
34	13.736	1935	1938	1947	rBV3	85699	140650	7.59%	0.789%

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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-BF090518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.865	1956	1960	1963	rBV	1836052	1615036	87.15%	9.062%
36	14.054	1990	1992	1996	rBV	58558	64860	3.50%	0.364%
37	14.365	2042	2045	2049	rBV3	78926	126865	6.85%	0.712%
38	14.630	2087	2090	2093	rBV	193348	213259	11.51%	1.197%
39	15.277	2195	2200	2204	rVB	916729	1115134	60.17%	6.257%

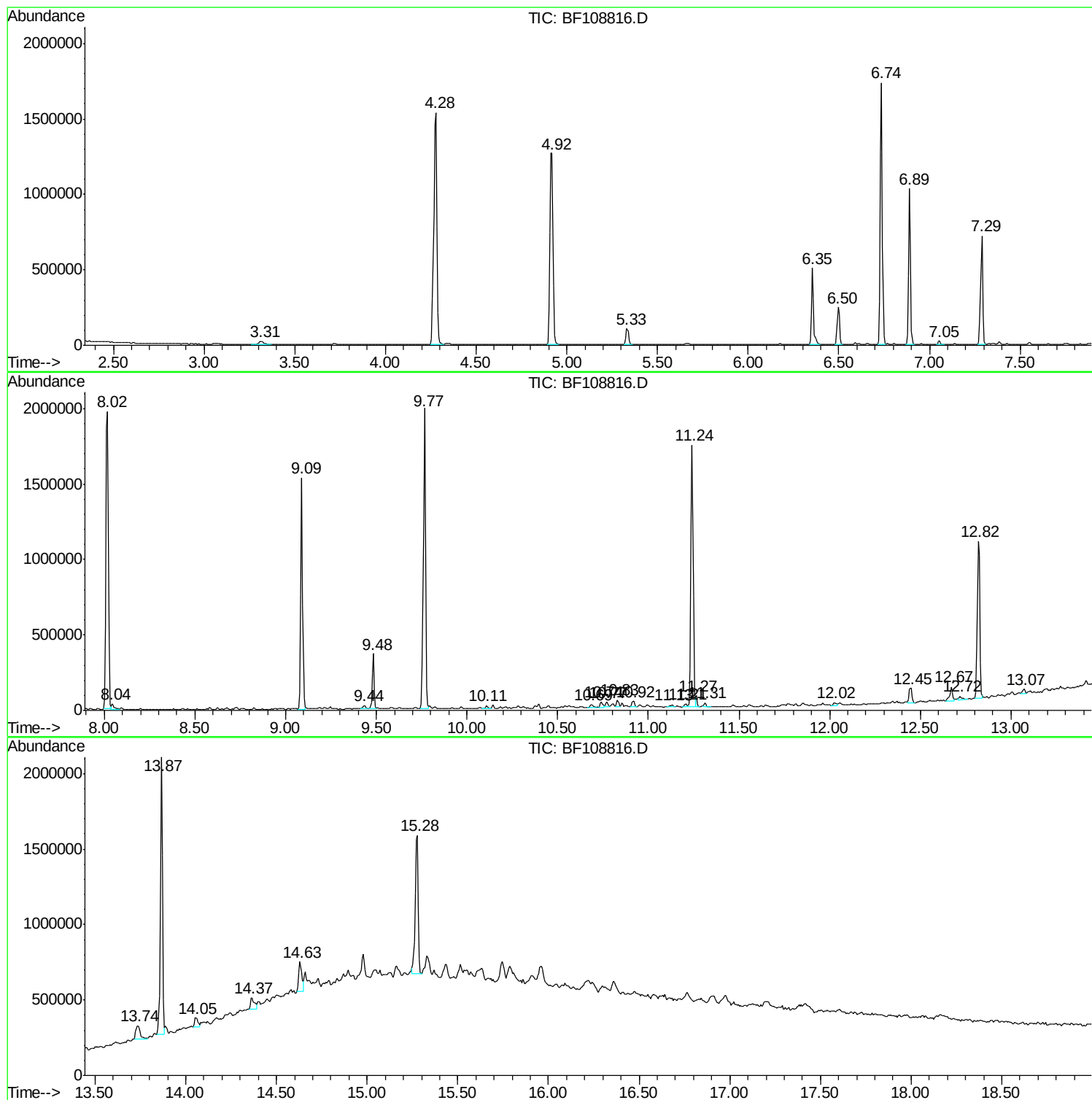
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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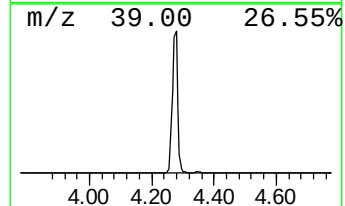
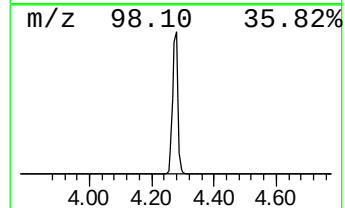
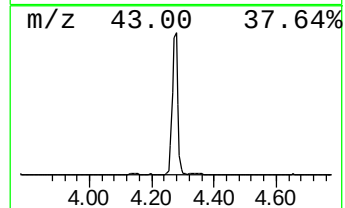
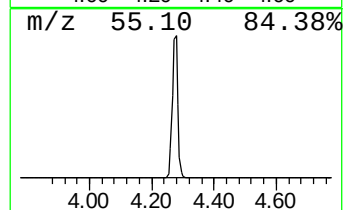
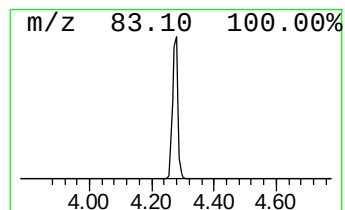
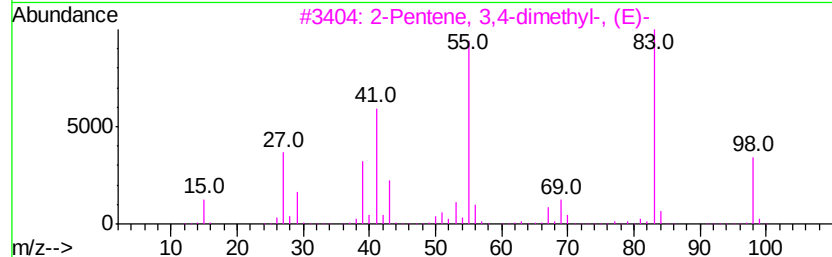
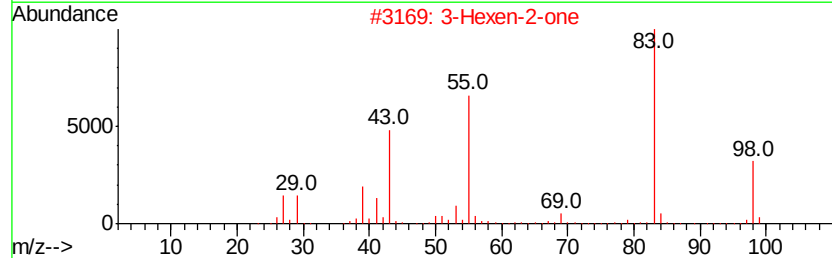
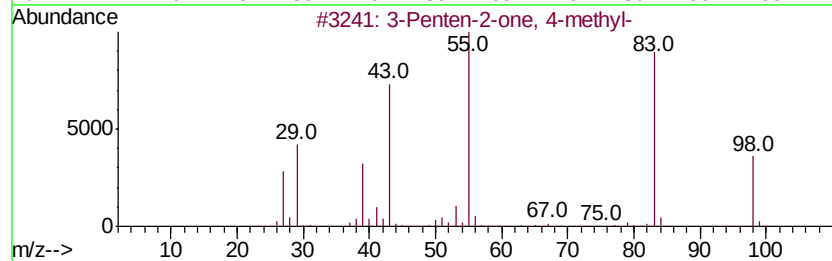
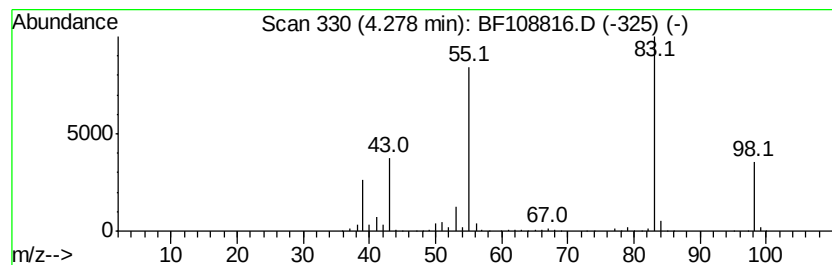
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	26.23 ng	1853200	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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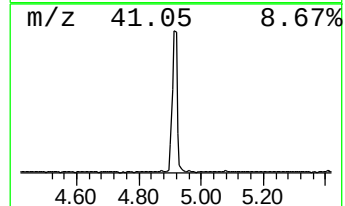
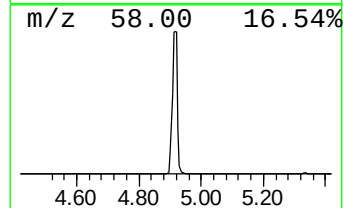
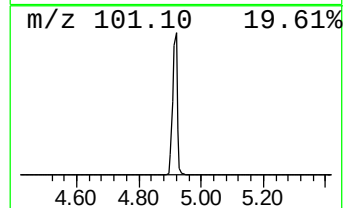
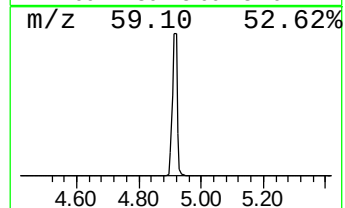
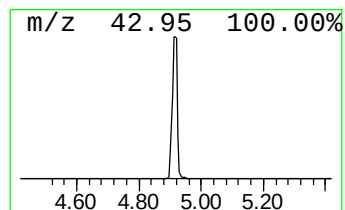
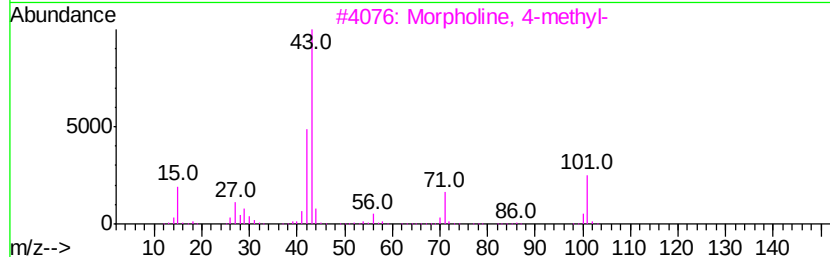
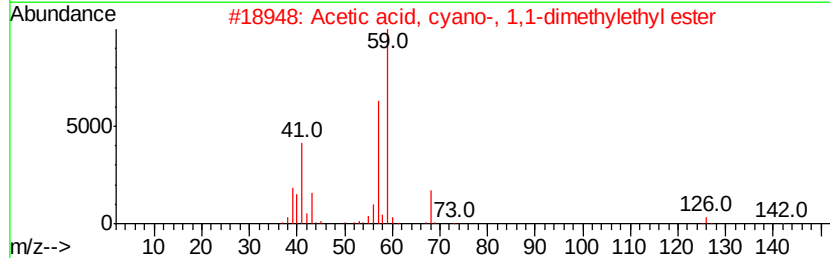
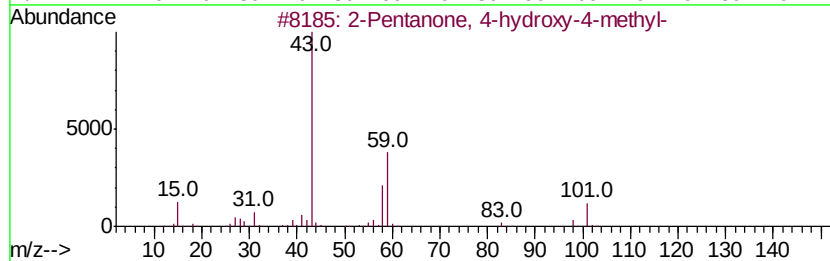
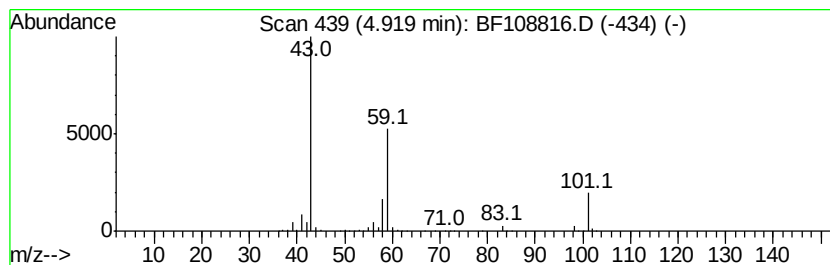
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	19.83 ng	1401060	1,4-Dichlorobenzene-d4	6.74

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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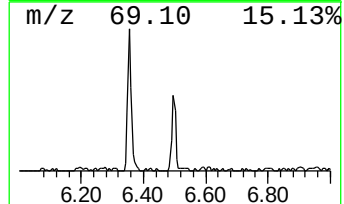
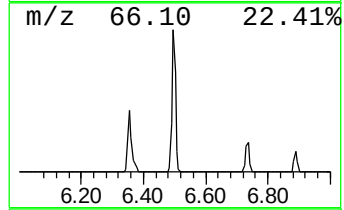
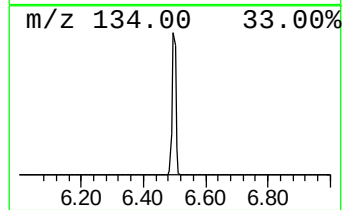
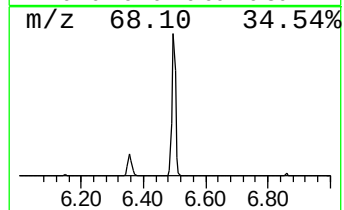
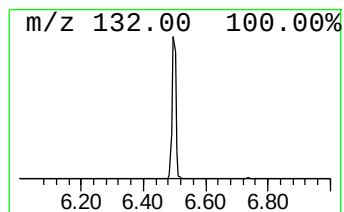
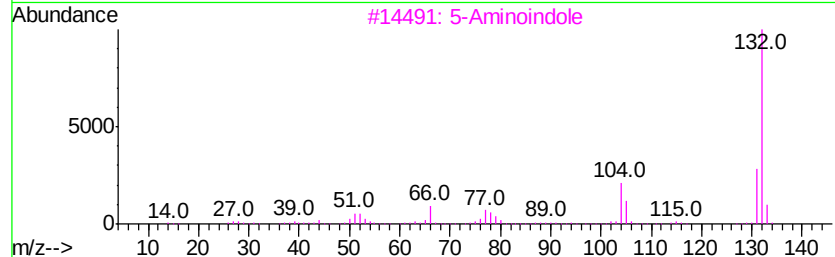
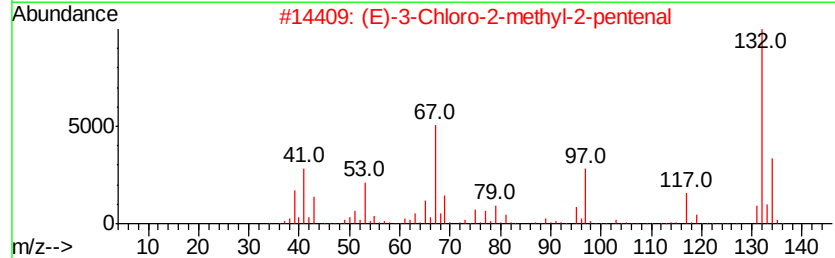
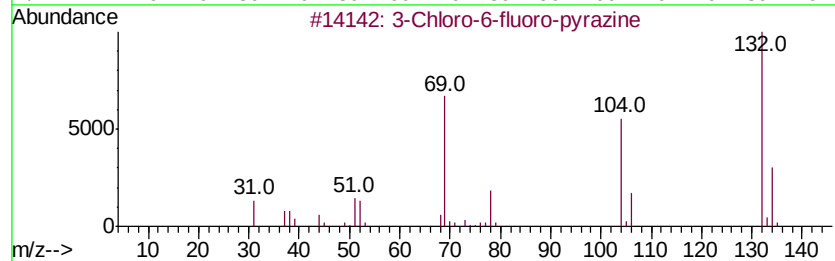
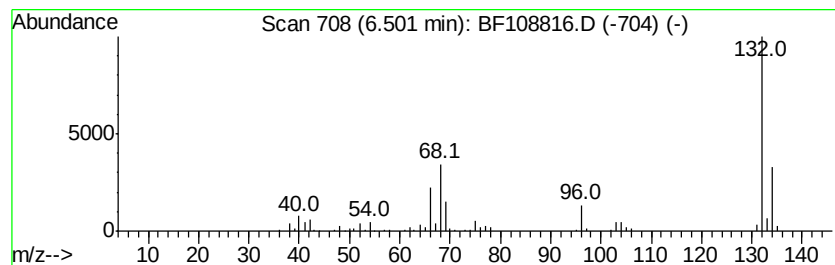
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.50 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	2.87 ng	202508	1,4-Dichlorobenzene-d4	6.74

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	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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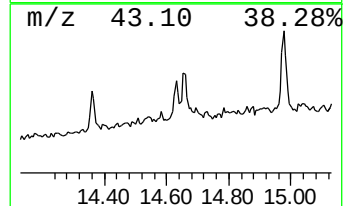
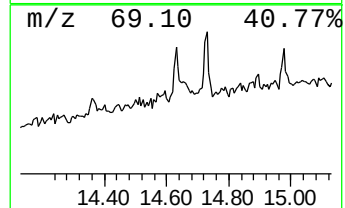
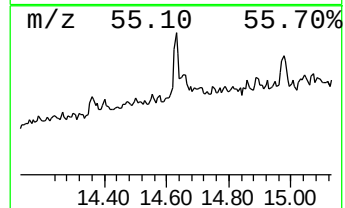
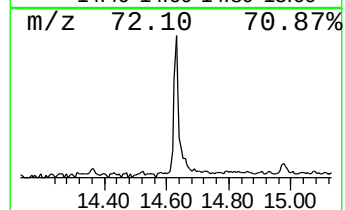
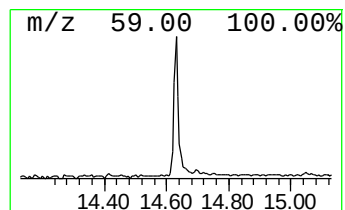
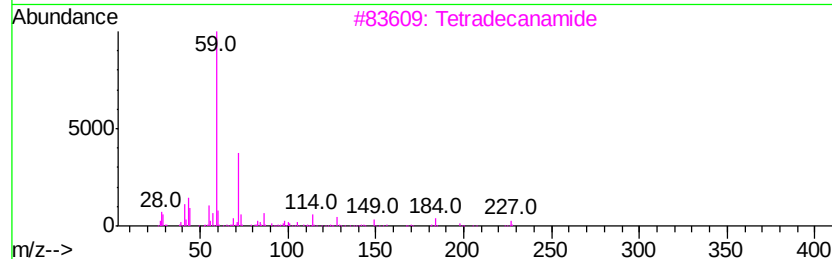
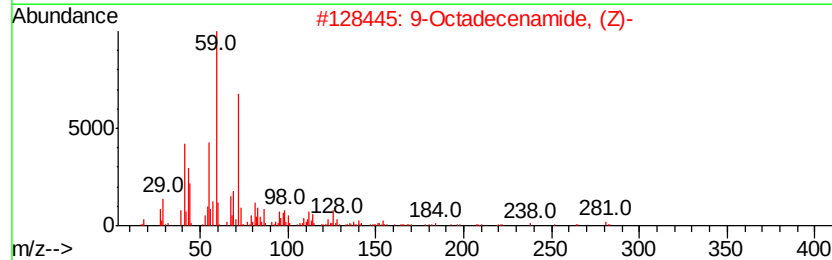
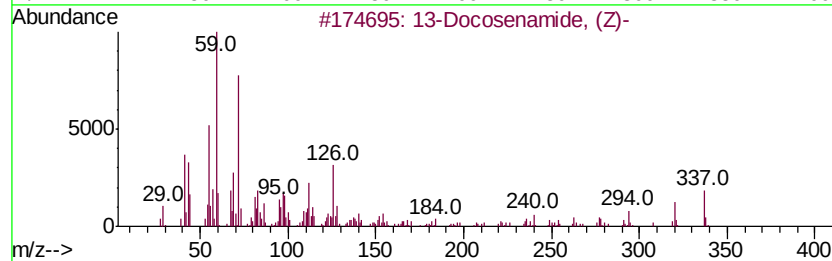
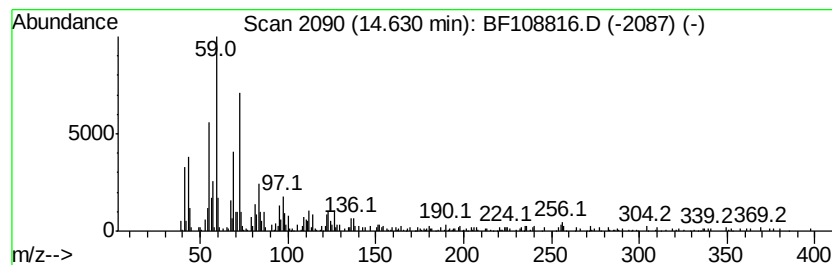
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.82 ng	213259	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3		Tetradecanamide	227	C14H29NO	000638-58-4	47
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5		N-Chloroacetyl-dl-erythro-0-meth...	209	C7H12ClNO4	1000214-48-1	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
3-Penten-2-one, 4...	4.28	26.2	ng	1853200	1	6.74	1412930	20.0
2-Pentanone, 4-hy...	4.92	19.8	ng	1401060	1	6.74	1412930	20.0
unknown6.50	6.50	2.9	ng	202508	1	6.74	1412930	20.0
13-Docosenamide, ...	14.63	3.8	ng	213259	6	15.28	1115130	20.0