

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
 Data File : BF108365.D
 Acq On : 22 Aug 2018 3:59
 Operator : JU/SJ
 Sample : J4516-06RE
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ND-BASELINE-WATERRE

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-BF080818.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	2.372	3	6	13	rVB	1390726	1842730	33.24%	5.015%
2	5.248	491	495	505	rVB	95709	112136	2.02%	0.305%
3	5.630	556	560	564	rBV	2361466	2133432	38.49%	5.806%
4	6.619	724	728	732	rBV	1516624	1384299	24.97%	3.767%
5	6.777	750	755	758	rBV	4136973	3933707	70.97%	10.705%
6	7.007	790	794	797	rBV	1127426	993562	17.92%	2.704%
7	7.166	816	821	824	rBV	4244726	3865340	69.73%	10.519%
8	7.571	884	890	893	rBV	3177680	3238574	58.43%	8.813%
9	8.289	1007	1012	1015	rBV	1380621	1166082	21.04%	3.173%
10	9.365	1188	1195	1198	rBV	6057817	5543002	100.00%	15.084%
11	9.754	1257	1261	1264	rBV	654542	548640	9.90%	1.493%
12	10.048	1307	1311	1315	rBV2	1332971	1220945	22.03%	3.323%
13	10.842	1442	1446	1450	rBV	2681581	2749740	49.61%	7.483%
14	11.548	1559	1566	1573	rBV	1107468	1269164	22.90%	3.454%
15	11.624	1576	1579	1582	rVB	114365	93958	1.70%	0.256%
16	11.736	1594	1598	1601	rBV	163880	132185	2.38%	0.360%
17	11.912	1624	1628	1631	rBV	336414	287796	5.19%	0.783%
18	12.330	1696	1699	1702	rBV	147183	113552	2.05%	0.309%
19	12.930	1798	1801	1803	rVB2	84781	71158	1.28%	0.194%
20	13.071	1822	1825	1830	rBV5	30837	58468	1.05%	0.159%
21	13.136	1831	1836	1839	rVV	3996067	3920471	70.73%	10.669%
22	13.595	1911	1914	1918	rBV4	43942	72979	1.32%	0.199%
23	13.912	1963	1968	1974	rBV9	41142	79889	1.44%	0.217%
24	14.200	2012	2017	2025	rVB	939958	990888	17.88%	2.697%
25	14.330	2037	2039	2046	rVB4	43521	62089	1.12%	0.169%
26	14.636	2088	2091	2096	rVB3	55474	80961	1.46%	0.220%
27	15.753	2275	2281	2287	rBV	560679	780727	14.08%	2.125%

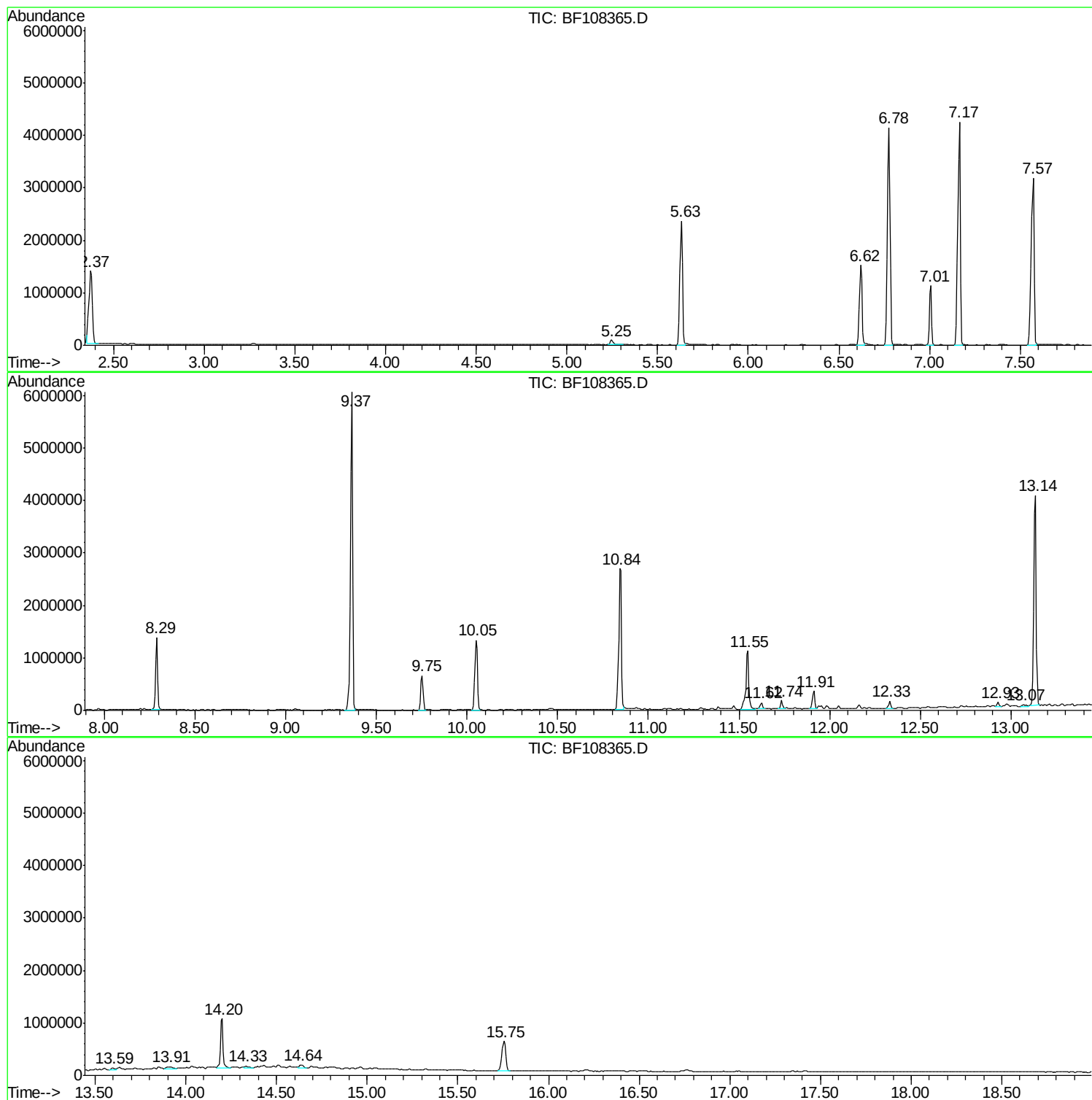
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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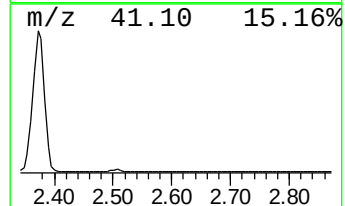
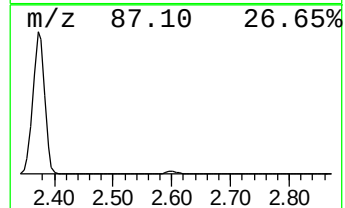
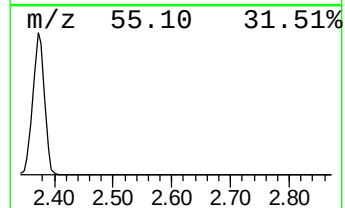
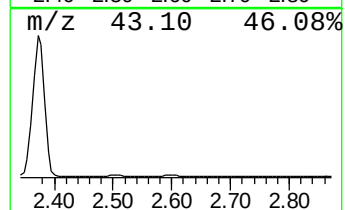
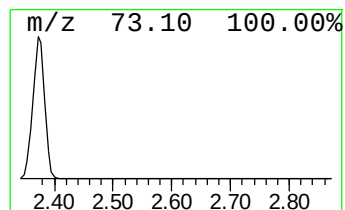
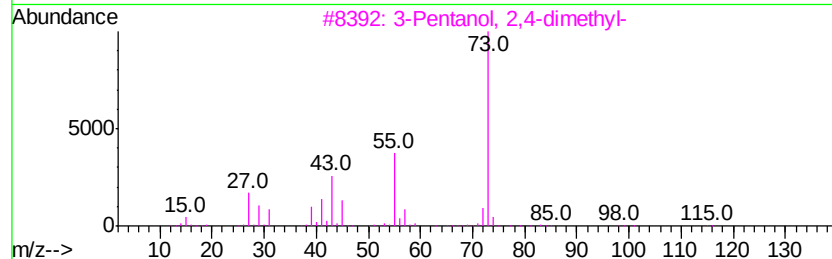
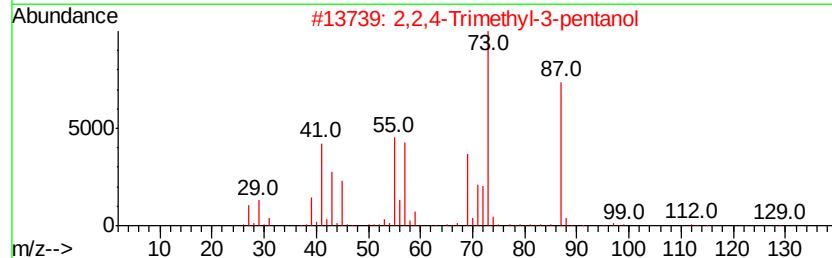
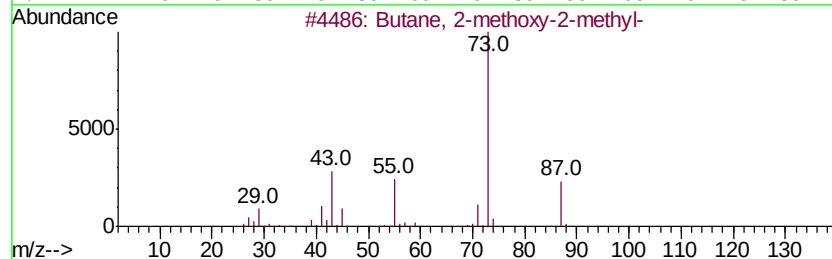
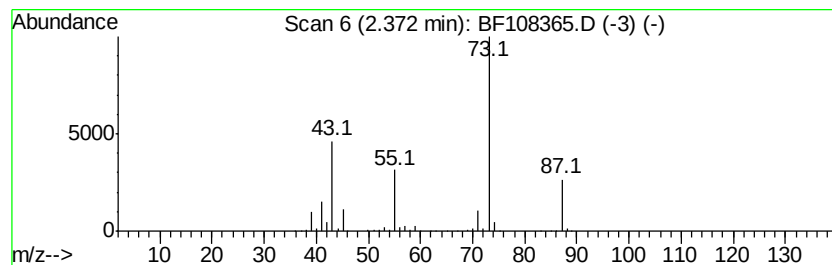
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	37.09 ng	1842730	1,4-Dichlorobenzene-d4	7.01

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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
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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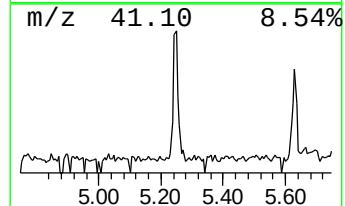
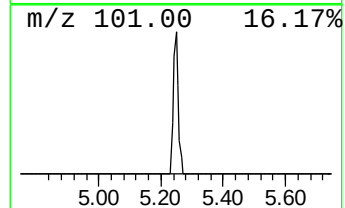
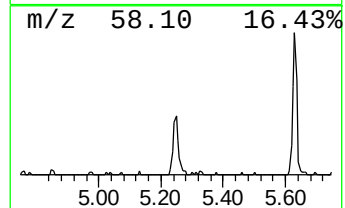
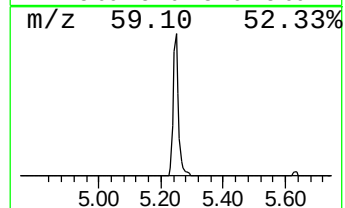
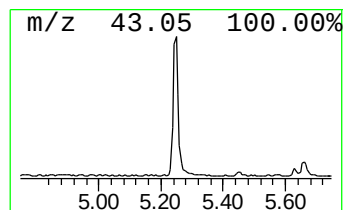
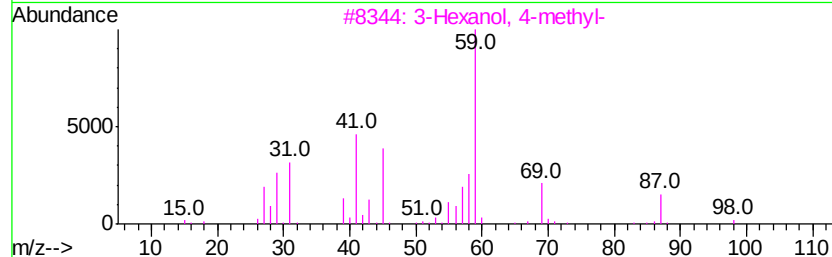
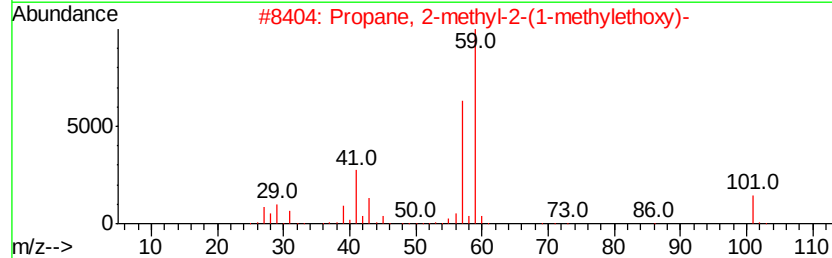
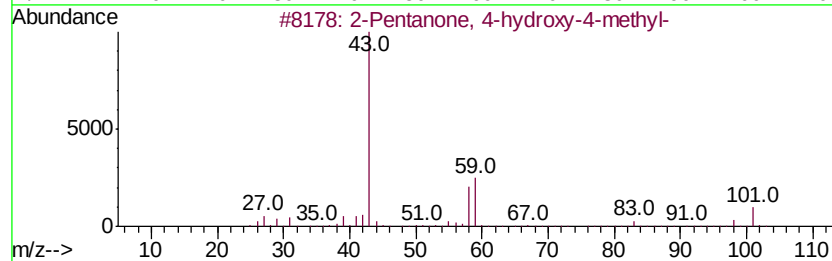
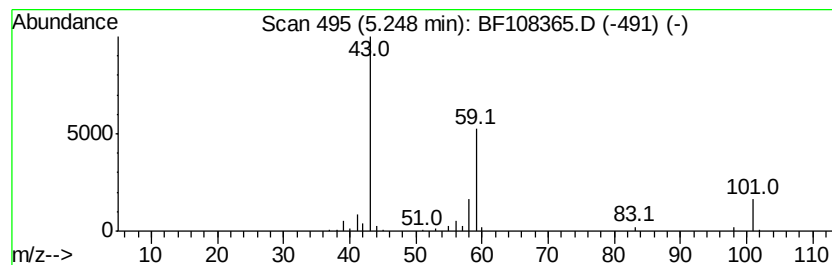
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.25	2.26 ng	112136	1,4-Dichlorobenzene-d4	7.01		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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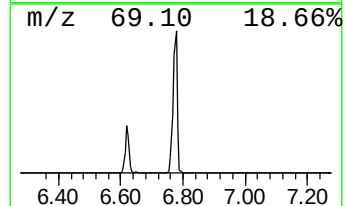
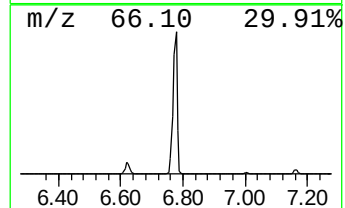
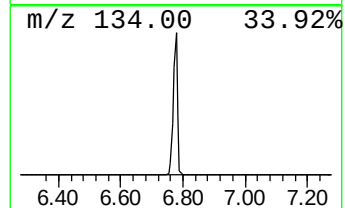
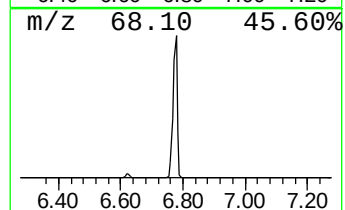
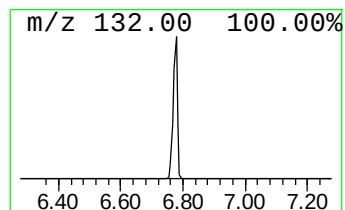
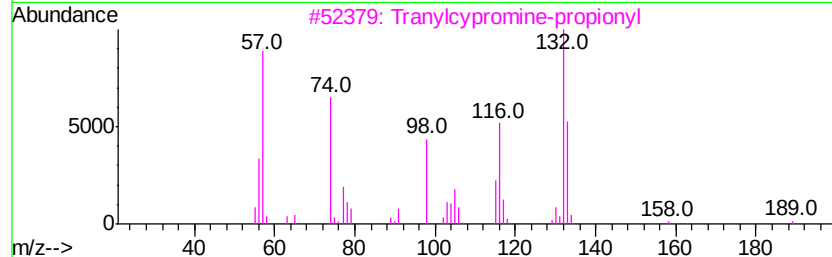
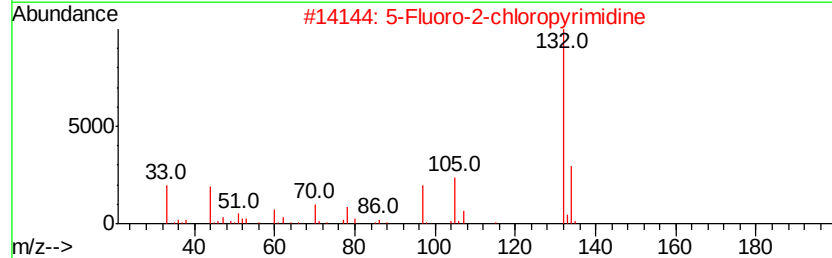
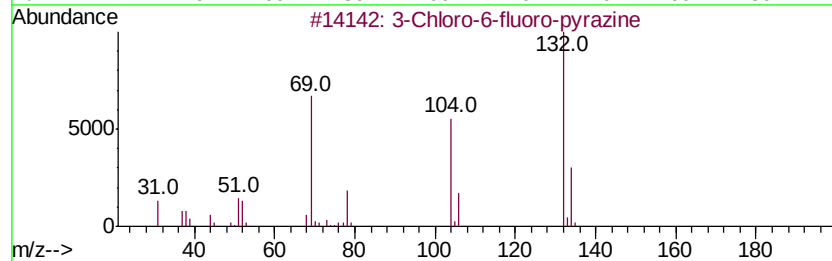
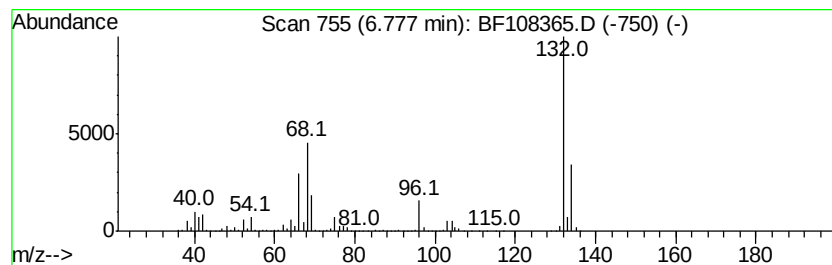
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Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	79.18 ng	3933710	1,4-Dichlorobenzene-d4	7.01

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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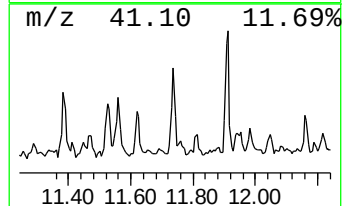
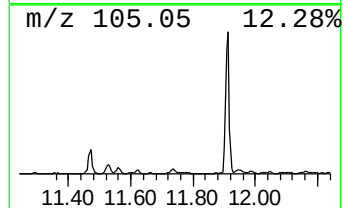
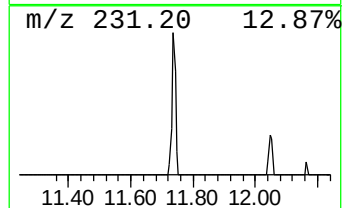
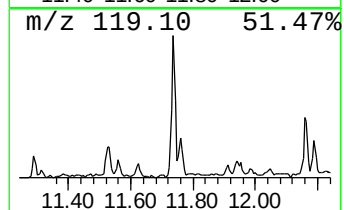
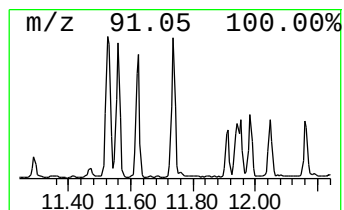
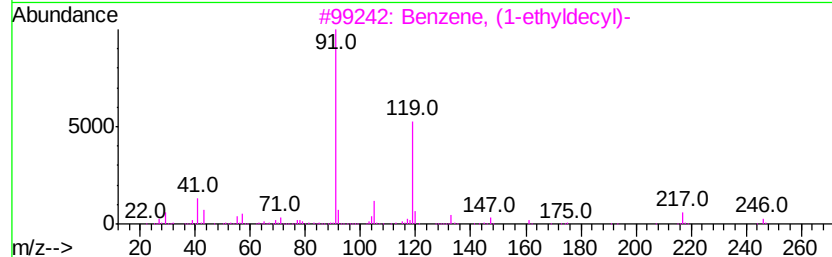
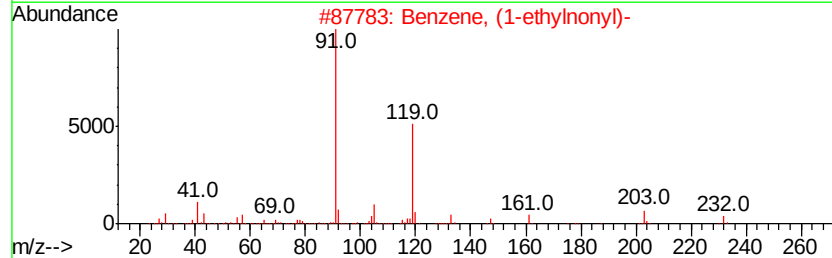
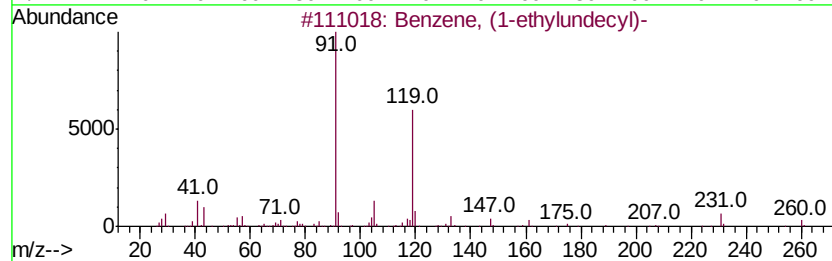
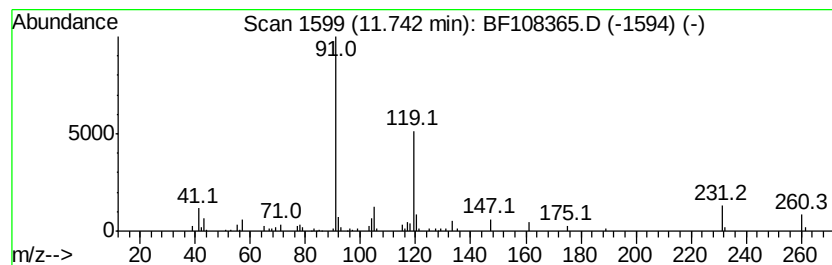
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Peak Number 5 Benzene, (1-ethylundecyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.08 ng	132185	Phenanthrene-d10	11.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	94
2		Benzene, (1-ethylnonyl)-	232	C17H28	004536-87-2	80
3		Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	72
4		Benzene, (1-ethyloctyl)-	218	C16H26	004621-36-7	64
5		Hexane, 3,4-diphenyl-	238	C18H22	005789-31-1	50



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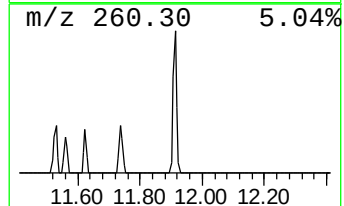
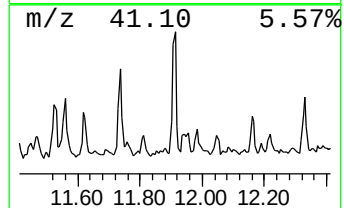
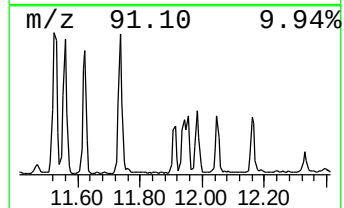
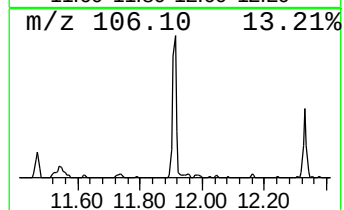
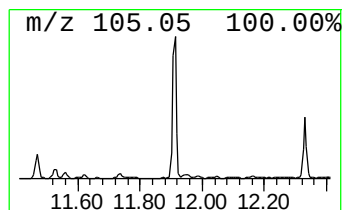
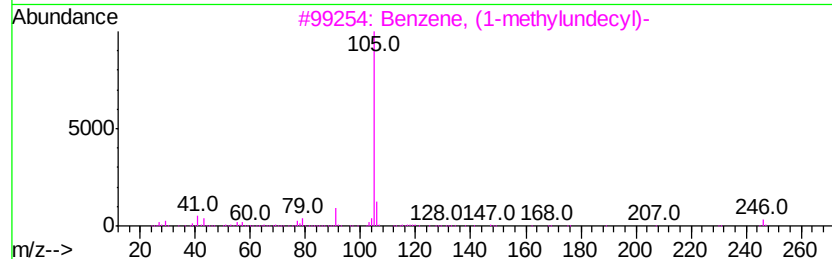
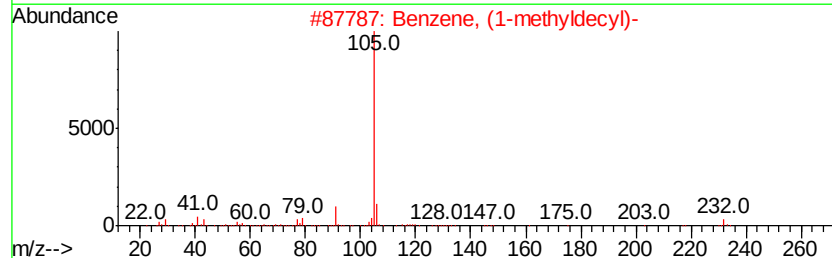
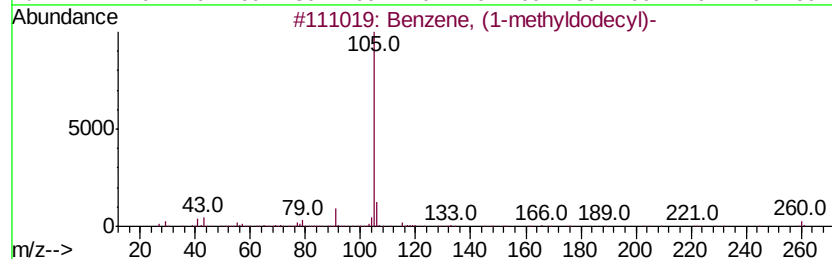
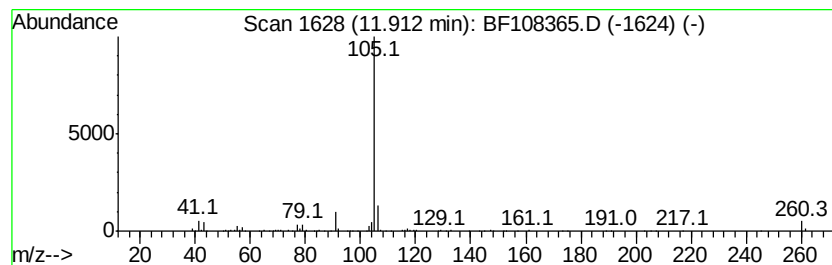
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Peak Number 6 Benzene, (1-methyldodecyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	4.54 ng	287796	Phenanthrene-d10	11.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	87
2		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
3		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	64
4		1-Hexene, 3-methyl-6-phenyl-4-(1...	294	C21H26O	1000194-52-4	64
5		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.37	37.1	ng	1842730	1	7.01	993562	20.0
2-Pentanone, 4-hy...	5.25	2.3	ng	112136	1	7.01	993562	20.0
unknown6.78	6.78	79.2	ng	3933710	1	7.01	993562	20.0
Benzene, (1-ethyl...	11.74	2.1	ng	132185	4	11.55	1269160	20.0
Benzene, (1-methy...	11.91	4.5	ng	287796	4	11.55	1269160	20.0