

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062018\
 Data File : BF106645.D
 Acq On : 21 Jun 2018 2:49
 Operator : JU/SJ
 Sample : J3554-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-3(5.0)

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-BF061918.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	5.207	484	488	496	rBV	152519	193403	8.79%	0.930%
2	5.607	552	556	560	rBV	2043930	1955230	88.85%	9.399%
3	6.607	721	726	732	rBV	1912749	2039114	92.66%	9.803%
4	6.742	744	749	752	rBV	2067983	2022382	91.90%	9.722%
5	6.960	782	786	789	rBV	645312	491412	22.33%	2.362%
6	7.119	808	813	816	rBV	1865008	1656567	75.28%	7.964%
7	7.525	877	882	885	rBV	1386670	1354590	61.56%	6.512%
8	7.983	957	960	963	rVB	74813	58712	2.67%	0.282%
9	8.242	1000	1004	1007	rBV	745822	604981	27.49%	2.908%
10	8.860	1104	1109	1112	rBV	1871686	1548078	70.35%	7.442%
11	9.319	1182	1187	1190	rBV	2437905	2200606	100.00%	10.579%
12	9.707	1249	1253	1259	rBV	490136	388789	17.67%	1.869%
13	10.001	1299	1303	1307	rBV2	721772	610666	27.75%	2.936%
14	10.413	1371	1373	1375	rVB	56907	38452	1.75%	0.185%
15	10.795	1434	1438	1441	rBV	1455548	1285400	58.41%	6.179%
16	10.883	1451	1453	1457	rBV	49708	49951	2.27%	0.240%
17	11.495	1553	1557	1560	rBV	626353	561549	25.52%	2.700%
18	12.877	1790	1792	1795	rBV	30428	27323	1.24%	0.131%
19	13.077	1822	1826	1829	rBV	2219815	2110839	95.92%	10.147%
20	13.289	1855	1862	1865	rBV3	16264	23865	1.08%	0.115%
21	13.583	1910	1912	1915	rVB	26058	23262	1.06%	0.112%
22	13.624	1915	1919	1922	rBV4	18332	24334	1.11%	0.117%
23	13.954	1972	1975	1981	rBV	134711	144715	6.58%	0.696%
24	14.142	2003	2007	2011	rBV	790693	687656	31.25%	3.306%
25	14.595	2081	2084	2088	rBV3	46755	57737	2.62%	0.278%
26	15.265	2196	2198	2203	rVB2	36705	43333	1.97%	0.208%
27	15.677	2263	2268	2273	rBV	414580	535591	24.34%	2.575%
28	16.130	2342	2345	2352	rVB	44284	63036	2.86%	0.303%

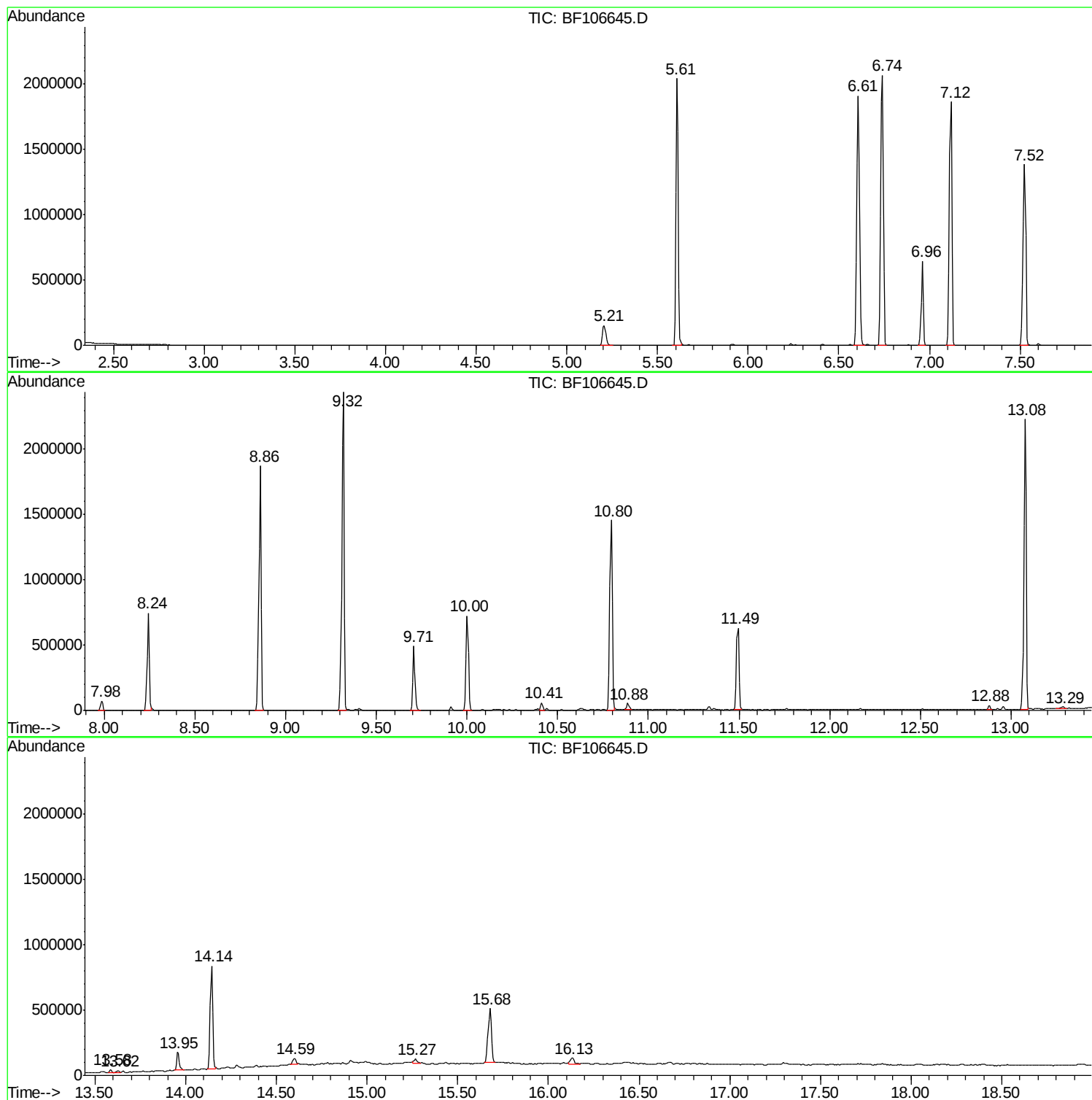
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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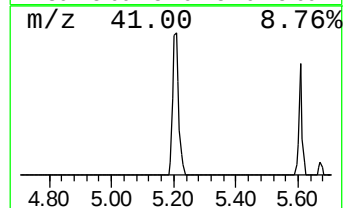
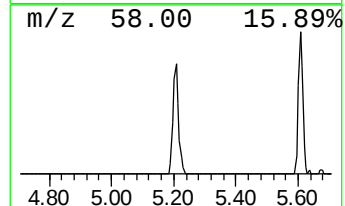
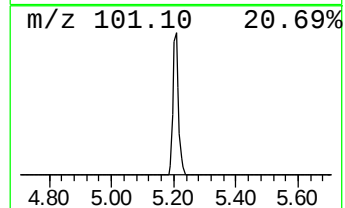
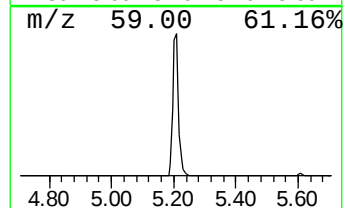
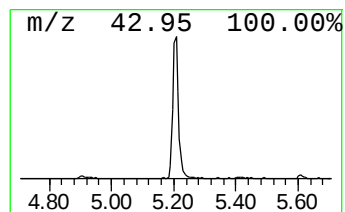
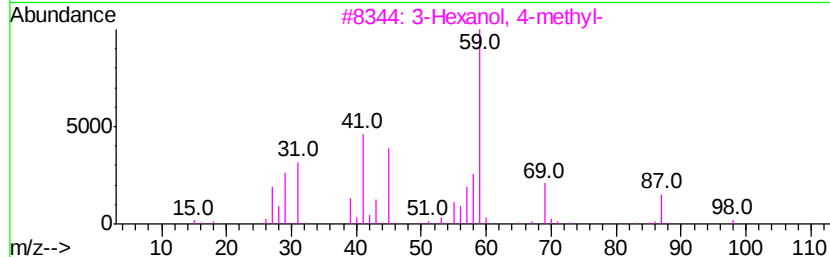
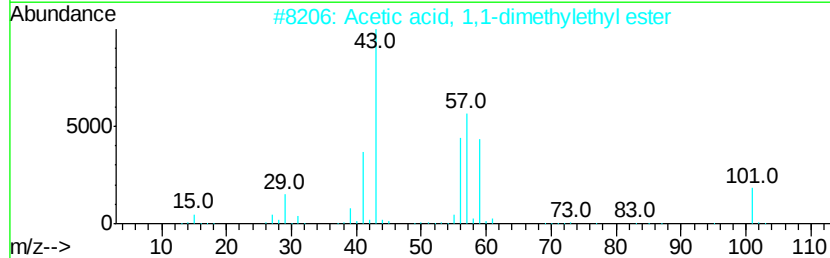
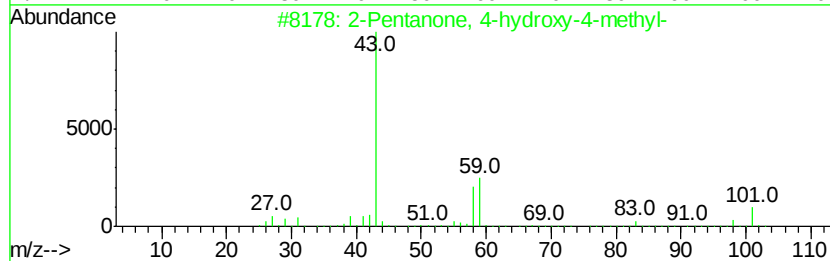
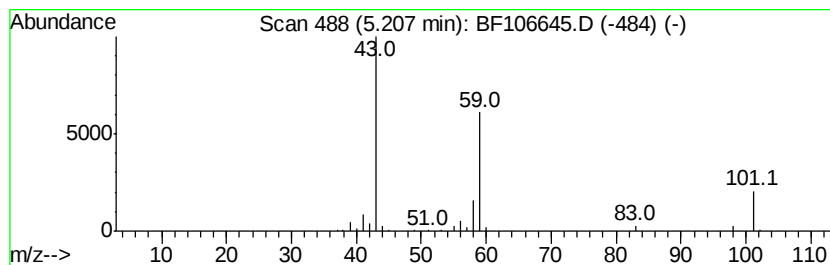
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	7.87 ng	193403	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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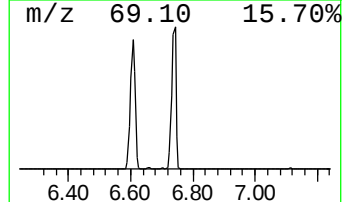
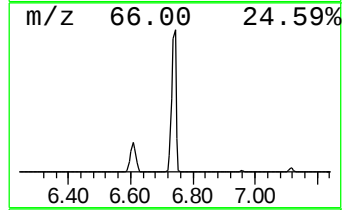
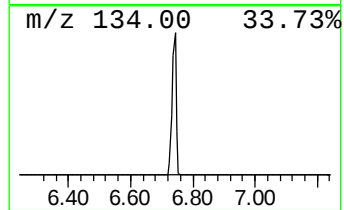
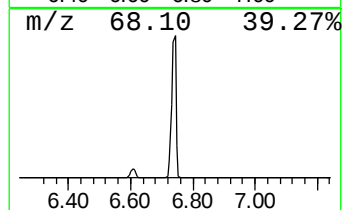
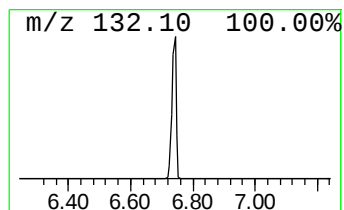
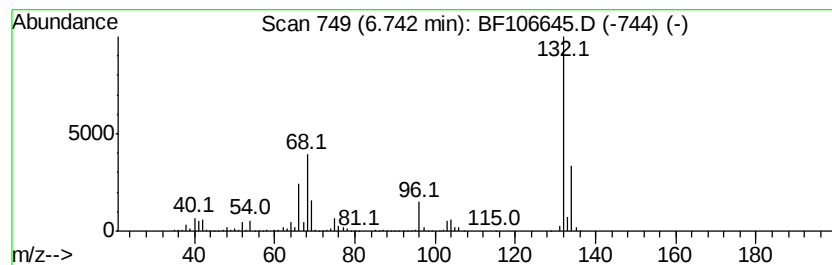
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	82.31 ng	2022380	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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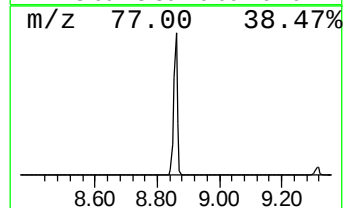
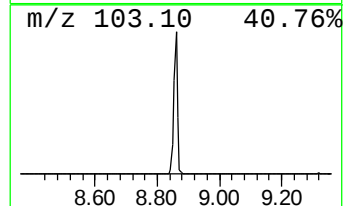
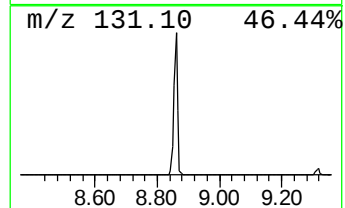
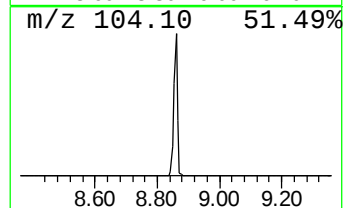
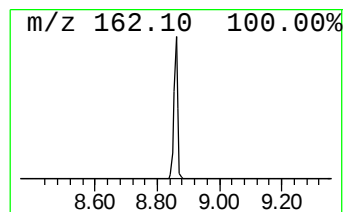
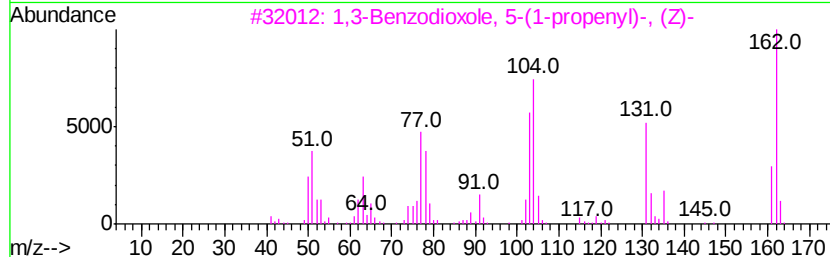
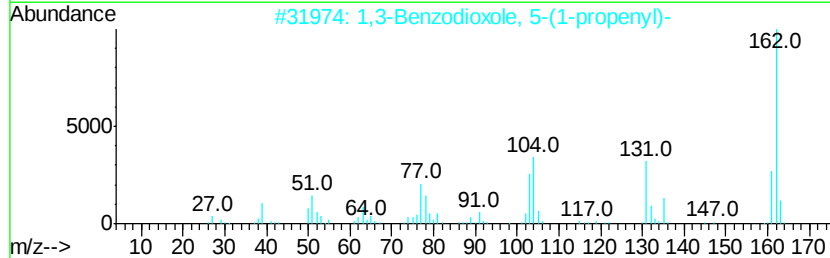
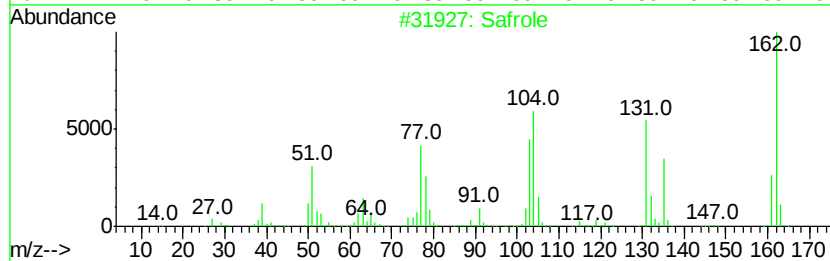
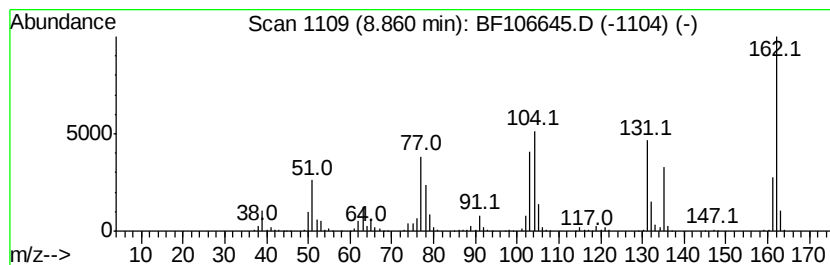
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Peak Number 4 Safrole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.86	51.18 ng	1548080	Napthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Safrole	162	C10H10O2	000094-59-7	98
2		1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3		1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	94
4		Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	94
5		1,4-Dioxo-1,2,3,4-tetrahydrophth...	162	C8H6N2O2	001445-69-8	41



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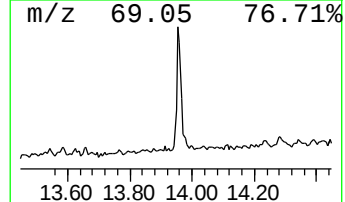
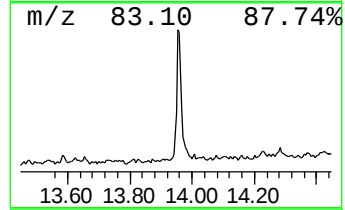
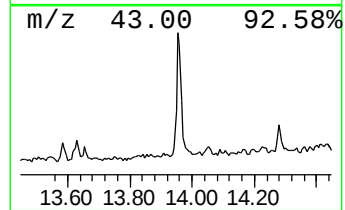
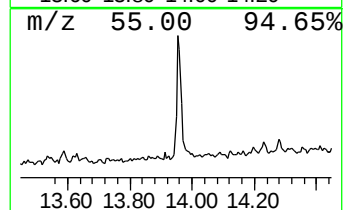
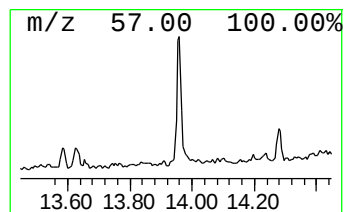
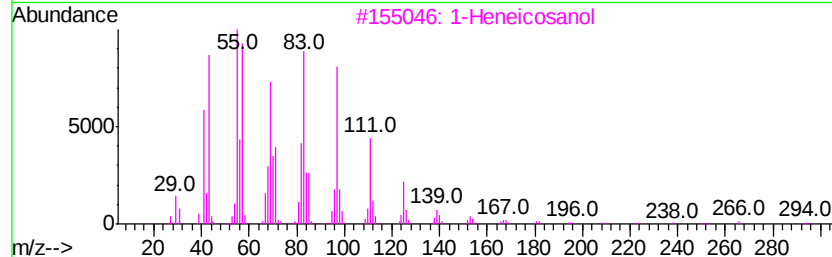
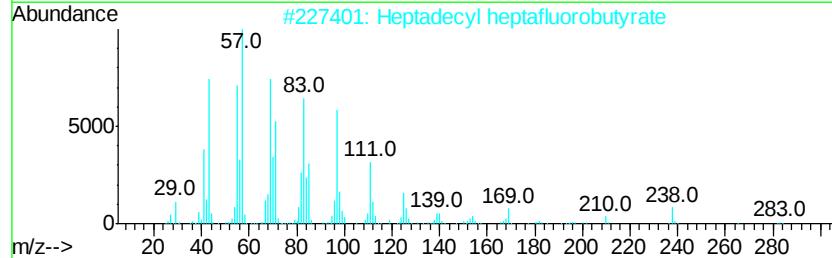
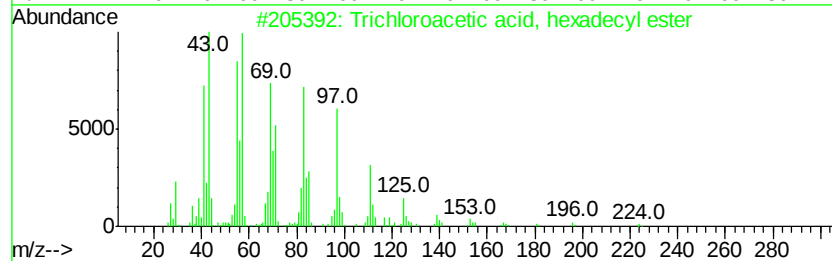
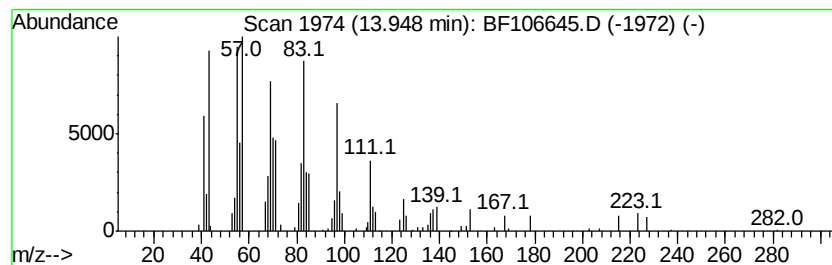
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.21 ng	144715	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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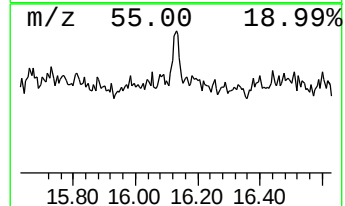
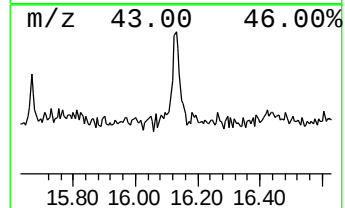
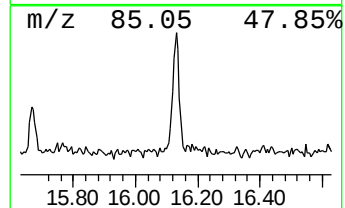
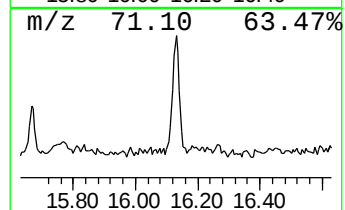
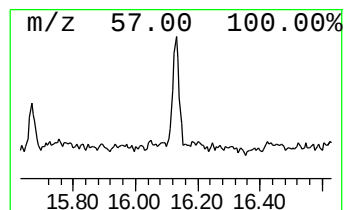
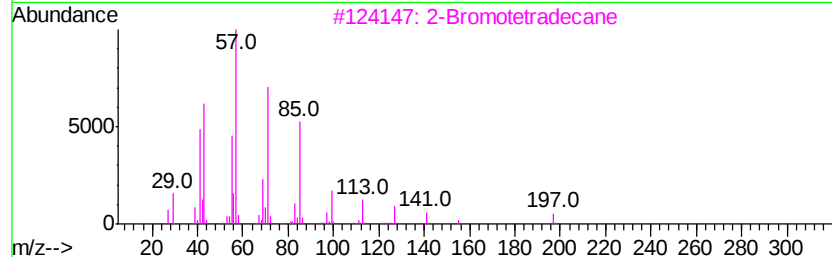
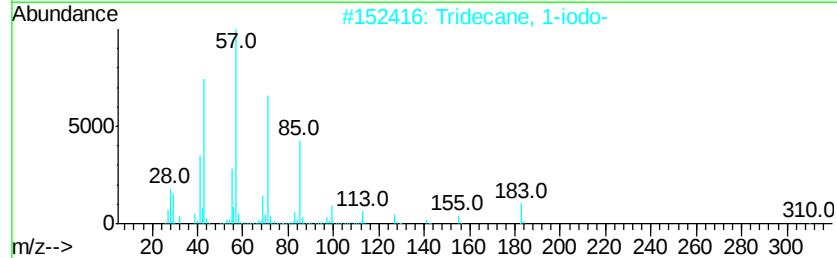
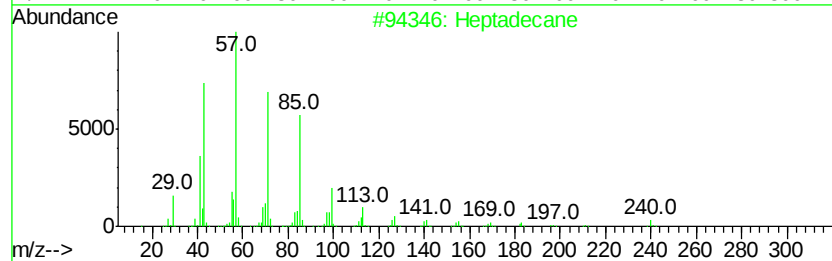
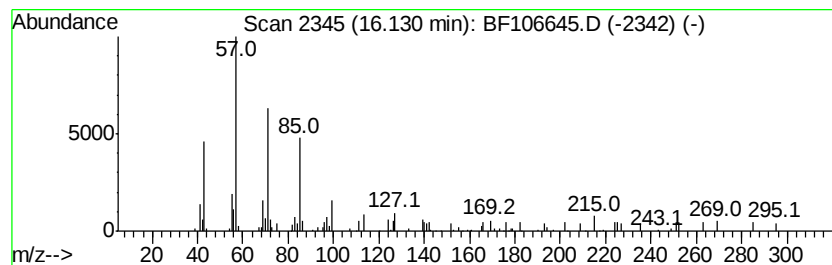
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.35 ng	63036	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	64
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	64
3	2-Bromotetradecane		276	C14H29Br	074036-95-6	59
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	59
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	7.9	ng	193403	1	6.96	491412	20.0
unknown6.74	6.74	82.3	ng	2022380	1	6.96	491412	20.0
Safole	8.86	51.2	ng	1548080	2	8.24	604981	20.0
Trichloroacetic a...	13.95	4.2	ng	144715	5	14.14	687656	20.0
Heptadecane	16.13	2.4	ng	63036	6	15.68	535591	20.0