

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071218\
 Data File : BF107348.D
 Acq On : 12 Jul 2018 19:20
 Operator : JU/SJ
 Sample : J3918-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-204-255-ETS

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-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	5.178	479	483	497	rBV	157471	294989	16.55%	1.781%
2	5.578	547	551	572	rBV	1491986	1677794	94.15%	10.131%
3	6.584	717	722	739	rBV	1405243	1780885	99.94%	10.754%
4	6.713	739	744	747	rVV	1582345	1621788	91.01%	9.793%
5	6.760	750	752	763	rVB	15091	21355	1.20%	0.129%
6	6.931	777	781	787	rBV	472402	392969	22.05%	2.373%
7	7.089	803	808	811	rBV	1368260	1352738	75.91%	8.168%
8	7.501	872	878	881	rBV	1023662	1070073	60.05%	6.461%
9	8.213	995	999	1018	rBV	500041	460999	25.87%	2.784%
10	9.289	1175	1182	1190	rBV	1750640	1761192	98.83%	10.635%
11	9.395	1197	1200	1204	rVB	27069	26861	1.51%	0.162%
12	9.683	1245	1249	1259	rVB	316266	273365	15.34%	1.651%
13	9.978	1295	1299	1303	rBV2	491028	427744	24.00%	2.583%
14	10.777	1431	1435	1446	rBV	968772	968031	54.32%	5.845%
15	11.477	1550	1554	1556	rBV	489069	424303	23.81%	2.562%
16	11.501	1556	1558	1562	rVB	74416	60508	3.40%	0.365%
17	12.695	1758	1761	1765	rBV	145388	140788	7.90%	0.850%
18	12.907	1794	1797	1799	rBV2	35193	37919	2.13%	0.229%
19	12.930	1799	1801	1805	rVB	172609	138750	7.79%	0.838%
20	13.066	1819	1824	1827	rBV	1799619	1781955	100.00%	10.760%
21	13.154	1834	1839	1843	rBV5	11116	21098	1.18%	0.127%
22	13.260	1850	1857	1861	rBV	37890	52389	2.94%	0.316%
23	13.607	1912	1916	1918	rBV	27699	28364	1.59%	0.171%
24	13.883	1960	1963	1965	rBV	19528	18478	1.04%	0.112%
25	13.942	1969	1973	1978	rBV2	116295	170052	9.54%	1.027%
26	14.077	1992	1996	1999	rBV	117455	112338	6.30%	0.678%
27	14.136	2001	2006	2009	rVV2	578866	610839	34.28%	3.688%
28	14.160	2009	2010	2015	rVB	89034	59506	3.34%	0.359%
29	14.248	2022	2025	2028	rBV2	33518	37388	2.10%	0.226%
30	14.560	2076	2078	2082	rBV3	46161	51078	2.87%	0.308%
31	14.877	2129	2132	2135	rVB	32987	34601	1.94%	0.209%
32	14.954	2142	2145	2154	rVB	46213	65849	3.70%	0.398%
33	15.224	2186	2191	2197	rVB2	79711	154275	8.66%	0.932%
34	15.612	2253	2257	2262	rBV2	58091	95567	5.36%	0.577%

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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	15.671	2263	2267	2272	rBV	249014	334086	18.75%	2.017%
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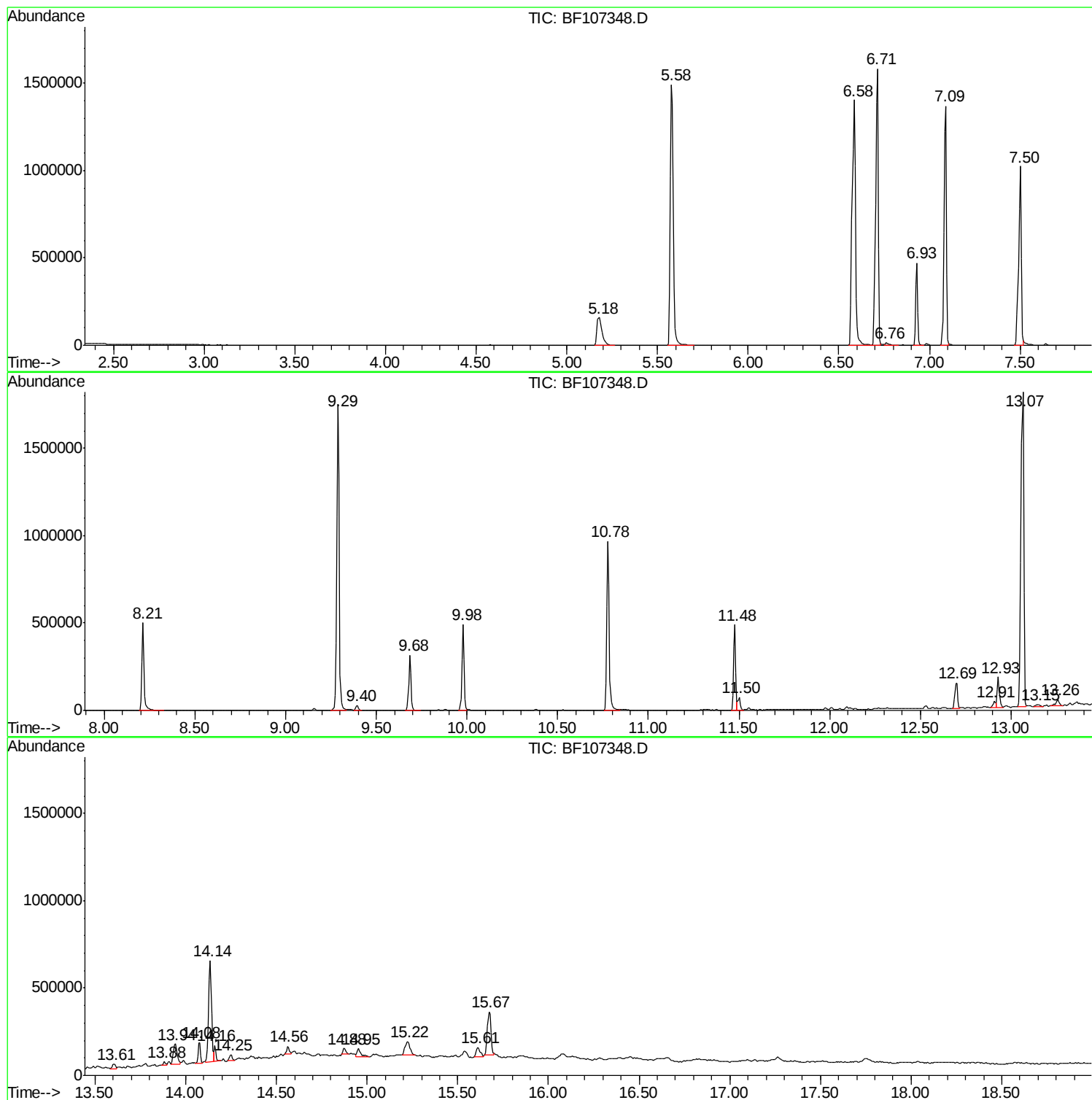
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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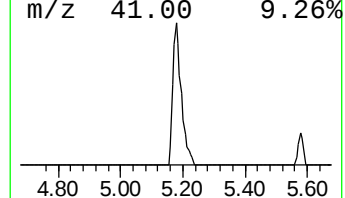
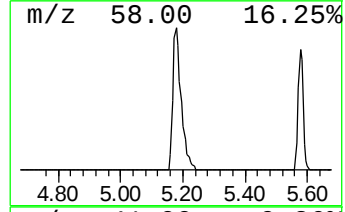
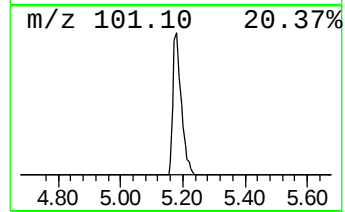
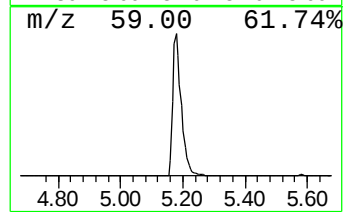
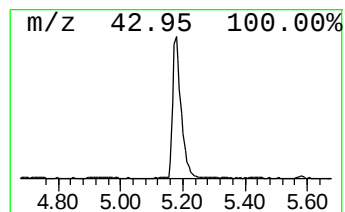
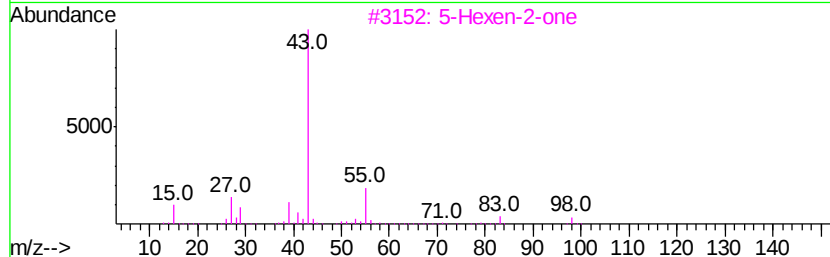
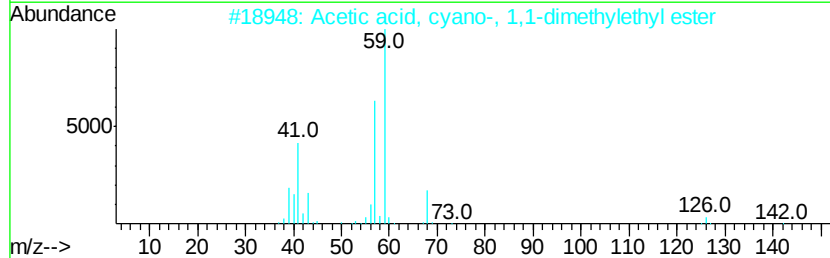
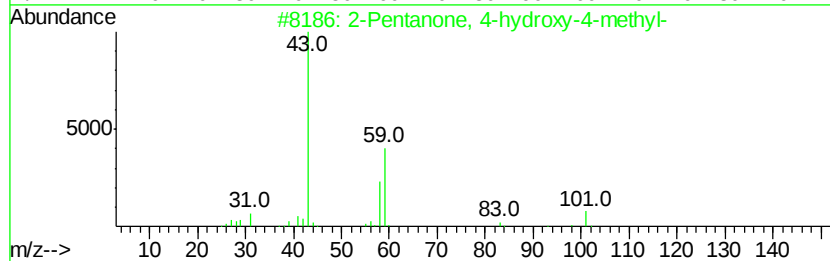
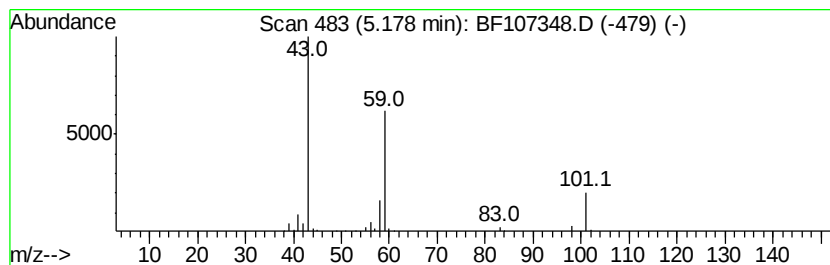
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	15.01 ng	294989	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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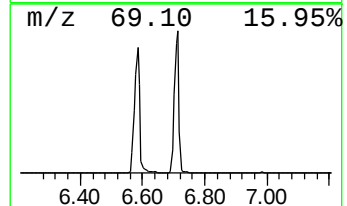
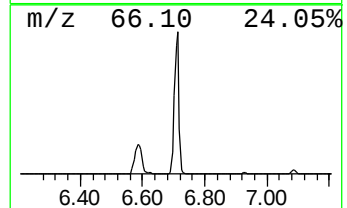
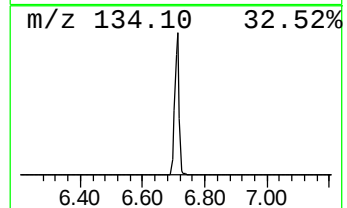
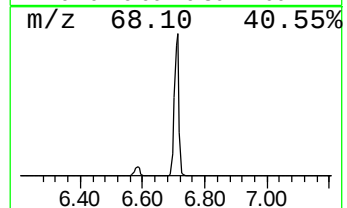
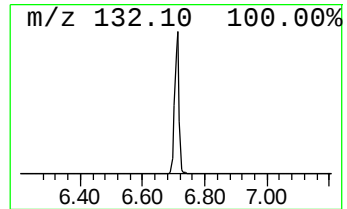
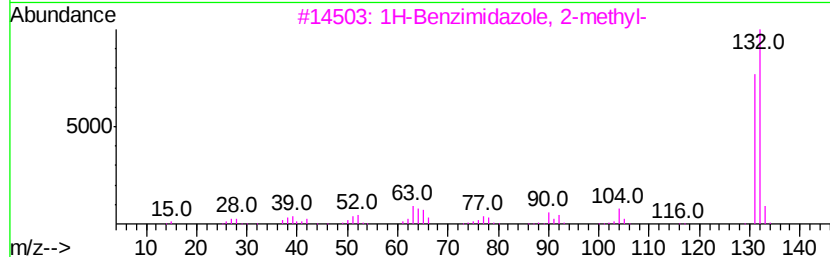
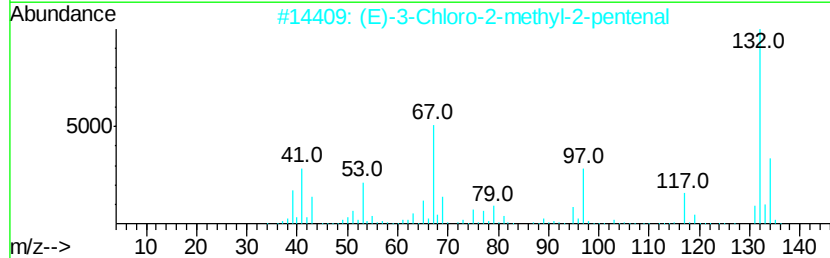
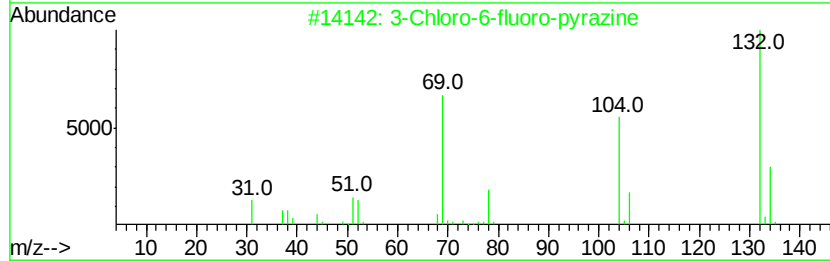
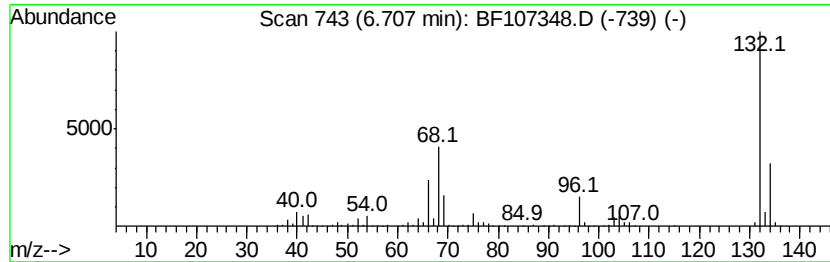
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	82.54 ng	1621790	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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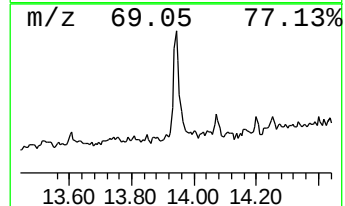
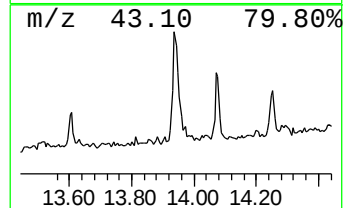
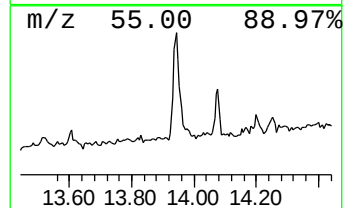
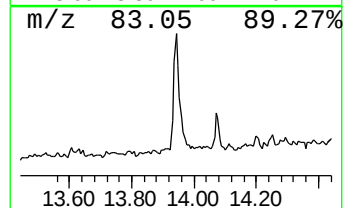
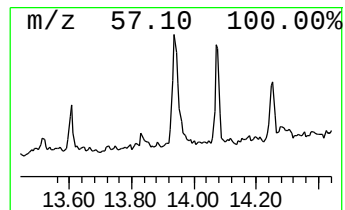
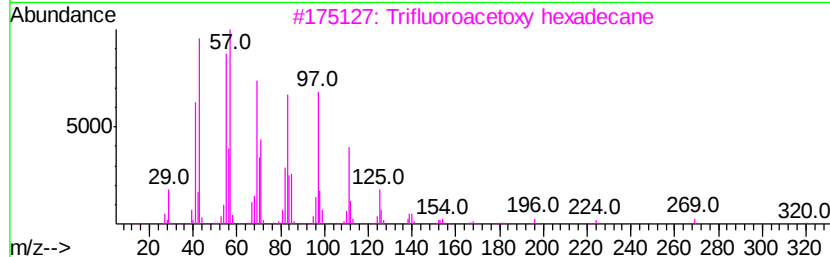
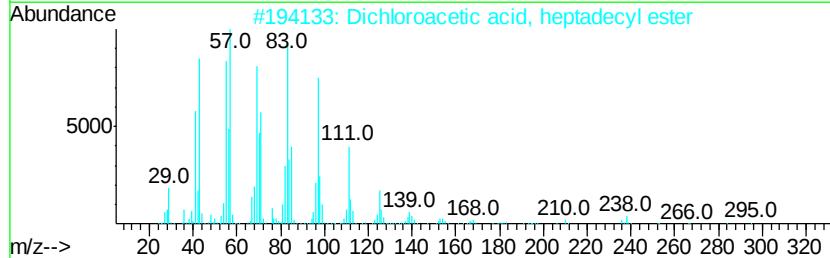
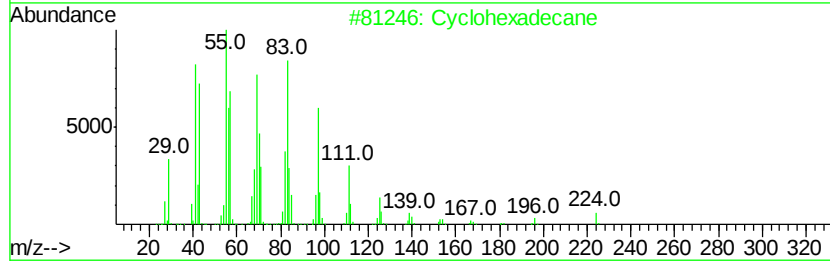
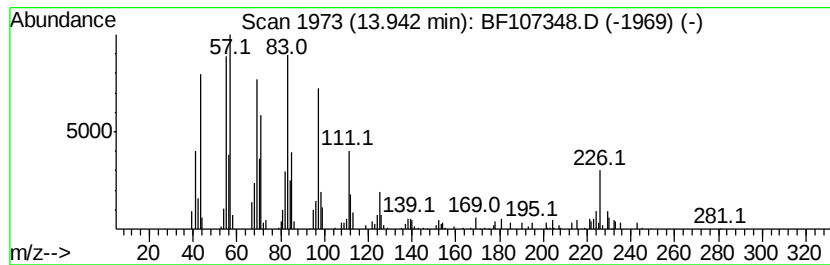
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Peak Number 4 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	5.57 ng	170052	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 97
2		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 90
3		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 87
4		Heptadecyl heptafluorobutyrte	452 C21H35F7O2	959085-66-6 86
5		n-Nonadecanol-1	284 C19H40O	001454-84-8 81



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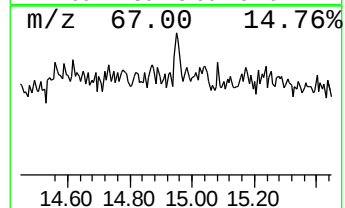
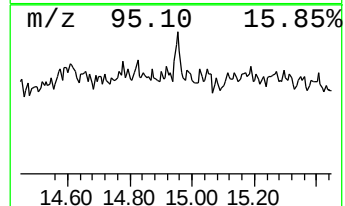
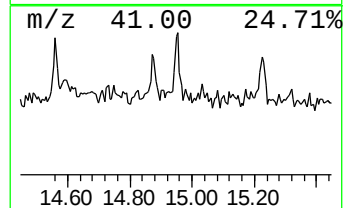
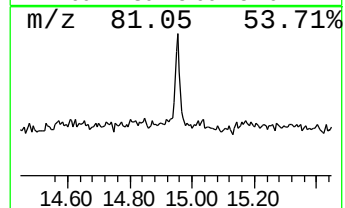
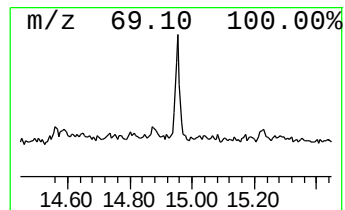
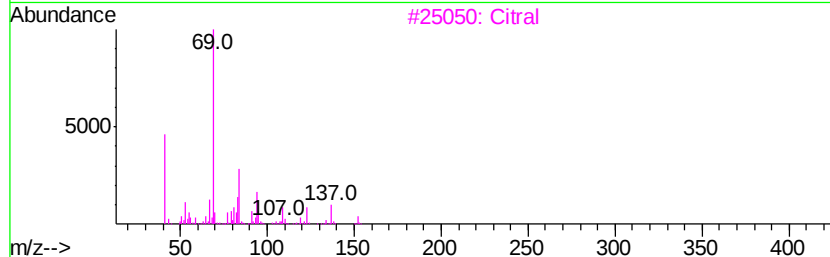
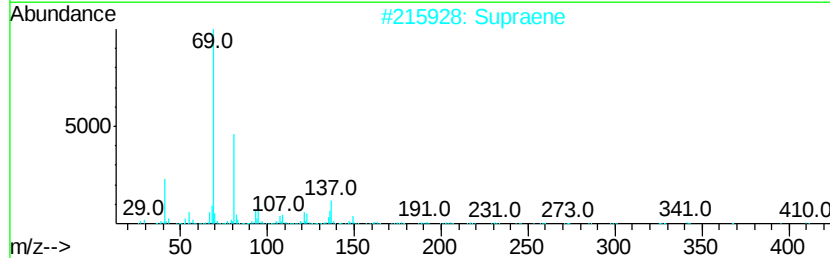
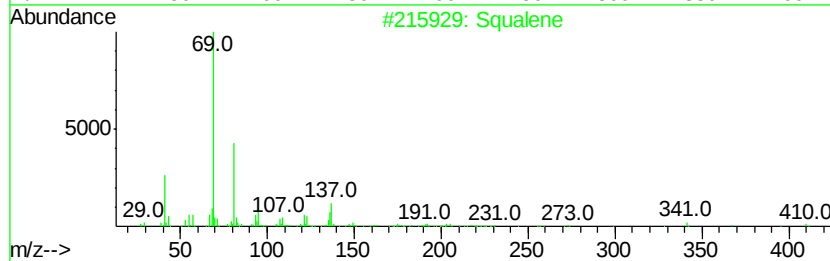
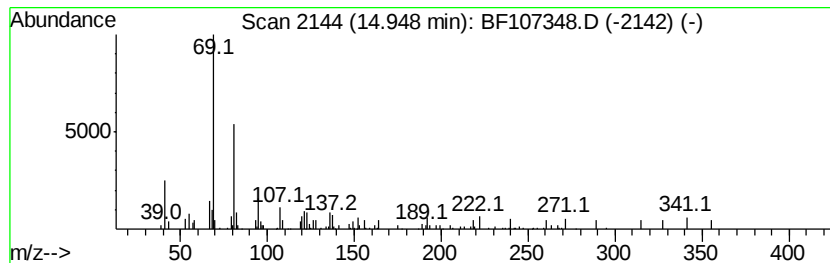
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.95	3.94 ng	65849	Perylene-d12	15.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	50
2	Supraene	410	C30H50	007683-64-9	49
3	Citral	152	C10H16O	005392-40-5	49
4	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	47
5	Farnesol, acetate	264	C17H28O2	1000352-67-2	47



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	15.0	ng	294989	1	6.93	392969	20.0
unknown6.71	6.71	82.5	ng	1621790	1	6.93	392969	20.0
Cyclohexadecane	13.94	5.6	ng	170052	5	14.14	610839	20.0
Squalene	14.95	3.9	ng	65849	6	15.67	334086	20.0