

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
 Data File : BF126361.D
 Acq On : 27 Dec 2021 18:04
 Operator : JU/CG
 Sample : M5218-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-C2

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126361.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.851	295	300	304	rVB	22874	29271	1.54%	0.200%
2	4.381	381	390	396	rBV	103873	125152	6.58%	0.854%
3	5.004	492	496	505	rVB	142508	159854	8.41%	1.090%
4	5.416	562	566	570	rBV	1605790	1426841	75.05%	9.733%
5	6.434	734	739	752	rBV	1954891	1901147	100.00%	12.969%
6	6.810	799	803	806	rBV	787299	639900	33.66%	4.365%
7	7.369	893	898	901	rBV	1371200	1184623	62.31%	8.081%
8	8.016	1002	1008	1017	rBV3	14843	40891	2.15%	0.279%
9	8.092	1017	1021	1024	rBV	954682	826416	43.47%	5.637%
10	9.169	1200	1204	1207	rBV	2197751	1849559	97.29%	12.617%
11	9.251	1215	1218	1224	rVB2	33563	34854	1.83%	0.238%
12	9.845	1315	1319	1323	rBV	1017242	809089	42.56%	5.519%
13	10.257	1386	1389	1391	rBV2	23038	23190	1.22%	0.158%
14	10.627	1449	1452	1460	rBV	590518	570881	30.03%	3.894%
15	11.227	1551	1554	1558	rVB	66650	59954	3.15%	0.409%
16	11.327	1568	1571	1574	rBV	770043	690344	36.31%	4.709%
17	11.351	1574	1575	1579	rVV	253021	169522	8.92%	1.156%
18	11.404	1582	1584	1589	rVB	31626	25460	1.34%	0.174%
19	11.498	1597	1600	1606	rVB	20983	24272	1.28%	0.166%
20	11.745	1636	1642	1646	rVB3	15642	31198	1.64%	0.213%
21	11.833	1653	1657	1659	rBV	49788	44181	2.32%	0.301%
22	11.857	1659	1661	1665	rVV	51798	52930	2.78%	0.361%
23	11.898	1665	1668	1671	rVV	44841	46924	2.47%	0.320%
24	11.939	1671	1675	1678	rVV2	59261	67627	3.56%	0.461%
25	11.963	1678	1679	1684	rVB	39094	33260	1.75%	0.227%
26	12.127	1703	1707	1709	rBV2	19698	27298	1.44%	0.186%
27	12.151	1709	1711	1716	rVB2	31118	29590	1.56%	0.202%
28	12.315	1736	1739	1741	rBV3	20737	22811	1.20%	0.156%
29	12.380	1746	1750	1753	rBV3	24416	28636	1.51%	0.195%
30	12.463	1762	1764	1770	rVB3	29618	30647	1.61%	0.209%
31	12.539	1774	1777	1780	rBV	114352	100880	5.31%	0.688%
32	12.768	1811	1816	1820	rBV	201196	174219	9.16%	1.188%
33	12.915	1837	1841	1845	rBV	1408090	1221784	64.27%	8.335%
34	12.992	1850	1854	1862	rVV4	14469	23828	1.25%	0.163%
35	13.092	1865	1871	1877	rVB4	16710	34619	1.82%	0.236%
36	13.462	1928	1934	1937	rBV2	27241	37576	1.98%	0.256%

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37	13.604	1956	1958	1965	rVB2	23492	26689	1.40%	0.182%
38	13.715	1972	1977	1980	rBV5	16698	24634	1.30%	0.168%
39	13.810	1990	1993	1995	rBV2	24034	23865	1.26%	0.163%
40	13.839	1995	1998	2001	rVV	34820	38624	2.03%	0.263%
41	13.886	2001	2006	2012	rVV5	33367	78176	4.11%	0.533%
42	13.968	2015	2020	2023	rVV	652598	615834	32.39%	4.201%
43	13.992	2023	2024	2027	rVB	57552	34748	1.83%	0.237%
44	14.068	2032	2037	2040	rVB3	28080	33397	1.76%	0.228%
45	14.145	2047	2050	2053	rVB3	19824	20978	1.10%	0.143%
46	14.451	2098	2102	2105	rBV2	28223	31281	1.65%	0.213%
47	14.751	2149	2153	2157	rBV3	30181	38806	2.04%	0.265%
48	14.827	2163	2166	2168	rBV	20881	24156	1.27%	0.165%
49	14.992	2191	2194	2204	rVV2	34448	74192	3.90%	0.506%
50	15.086	2207	2210	2217	rVB3	31453	43797	2.30%	0.299%
51	15.292	2237	2245	2250	rVB3	30925	66648	3.51%	0.455%
52	15.351	2252	2255	2261	rVB	37666	45878	2.41%	0.313%
53	15.415	2261	2266	2270	rBV	521965	628179	33.04%	4.285%
54	15.462	2270	2274	2277	rVB3	31024	45229	2.38%	0.309%
55	15.762	2321	2325	2333	rVB2	24958	47317	2.49%	0.323%
56	15.892	2342	2347	2352	rBV	24365	40313	2.12%	0.275%
57	16.345	2421	2424	2428	rBV3	22470	34418	1.81%	0.235%
58	17.056	2540	2545	2551	rVB7	20331	42904	2.26%	0.293%

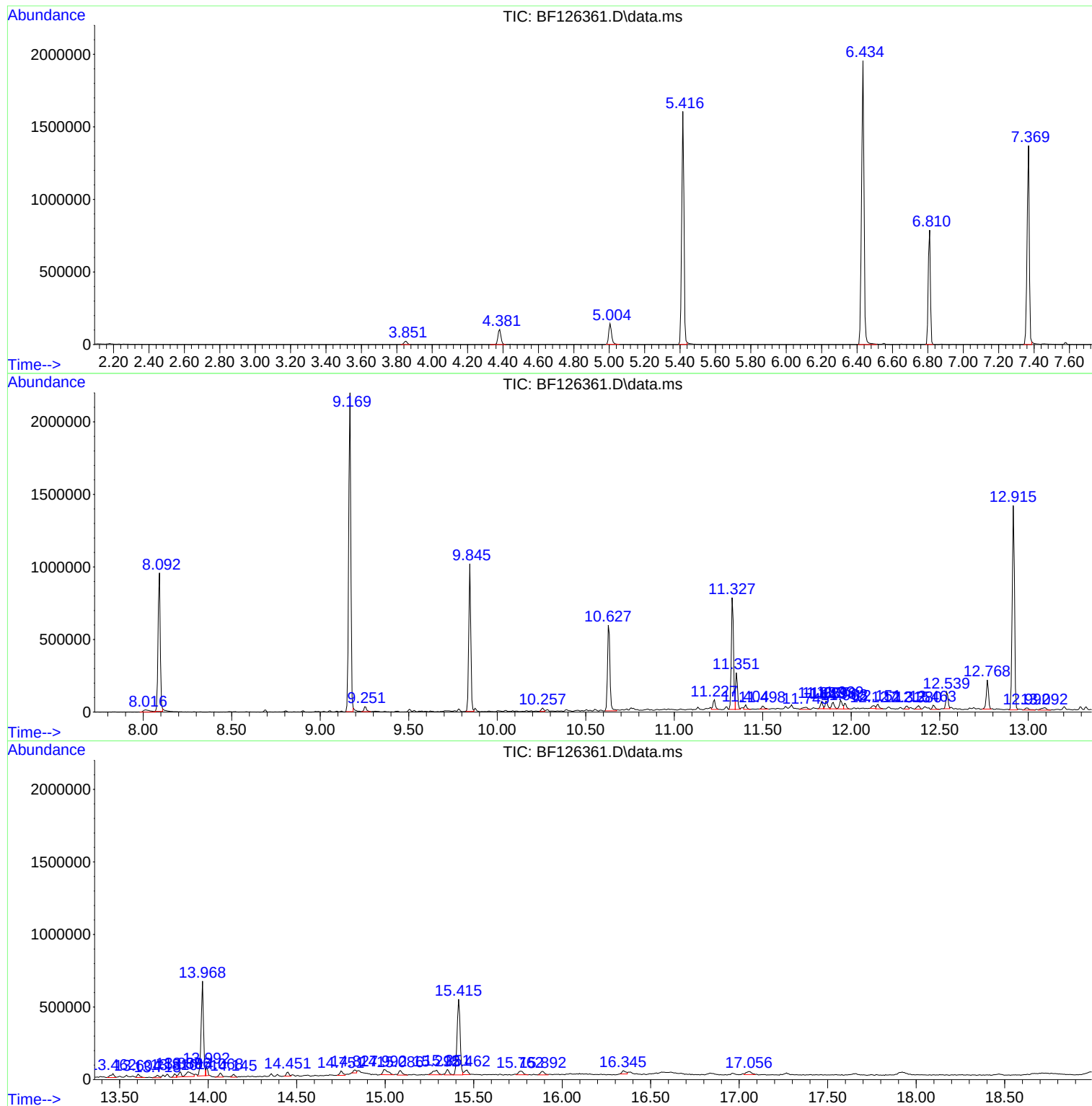
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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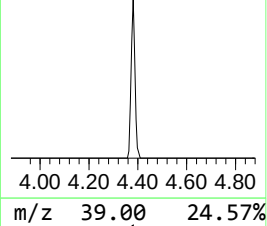
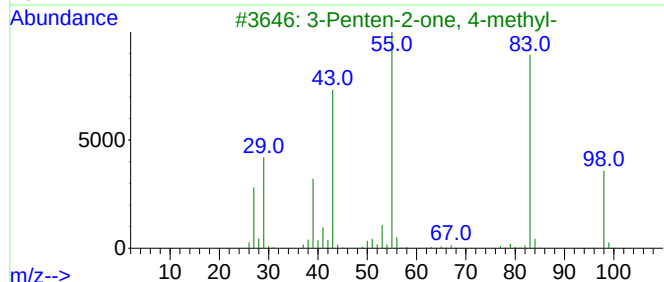
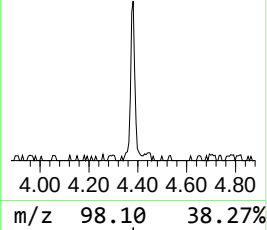
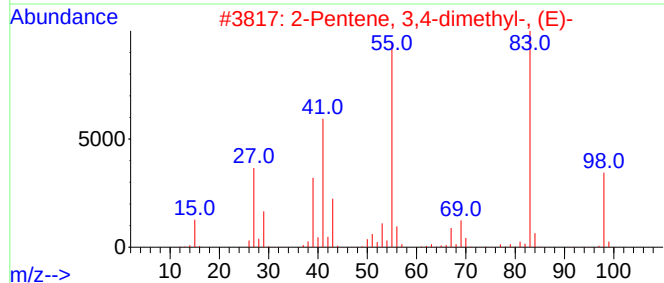
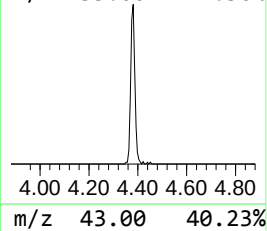
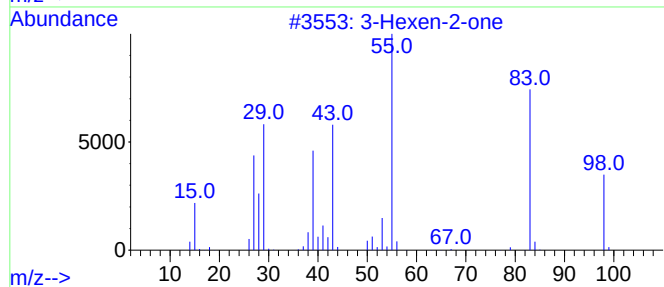
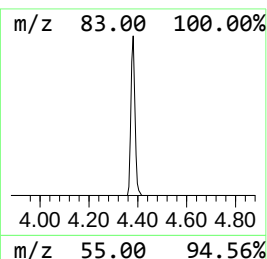
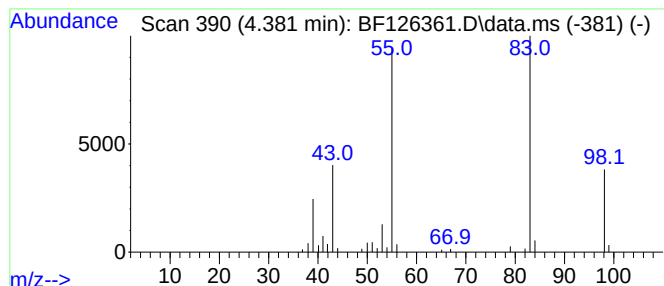
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.381	3.91 ng	125152	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			Cyclohexane, methyl-	98	C7H14	000108-87-2	80



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Instrument :
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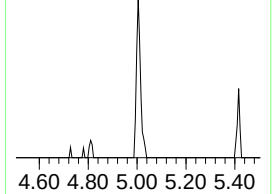
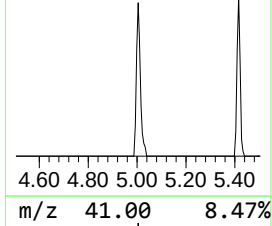
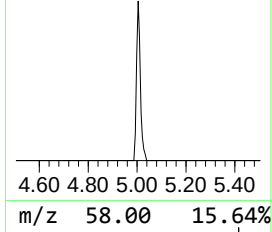
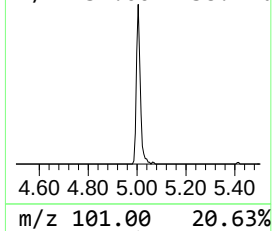
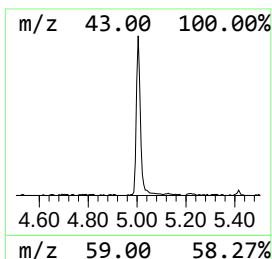
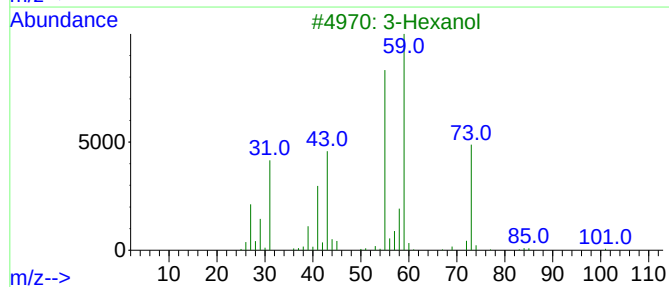
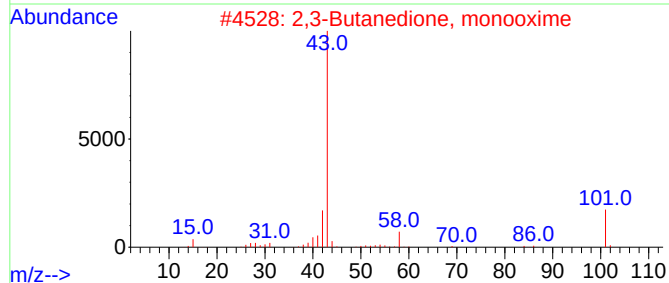
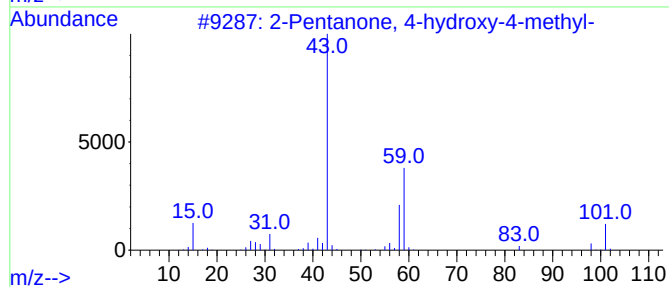
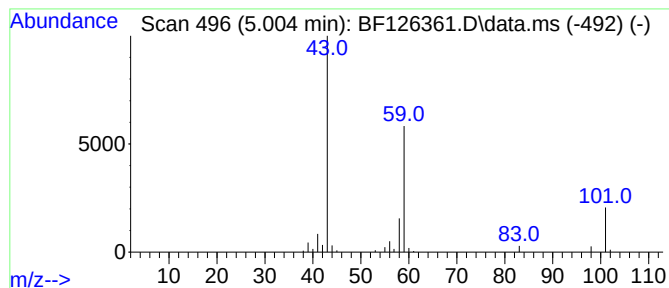
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	5.00 ng	159854	1,4-Dichlorobenzene-d4	6.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38	
3	3-Hexanol	102	C6H14O	000623-37-0	25	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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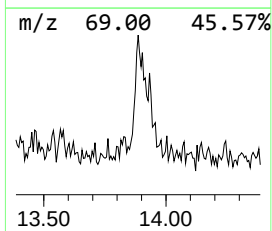
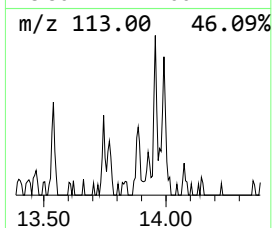
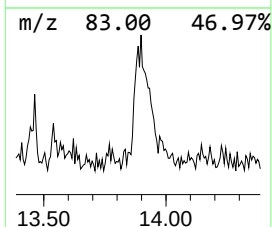
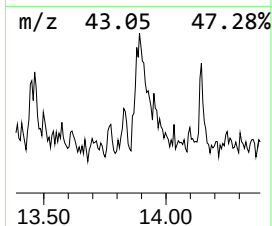
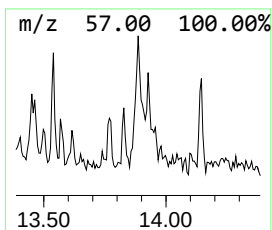
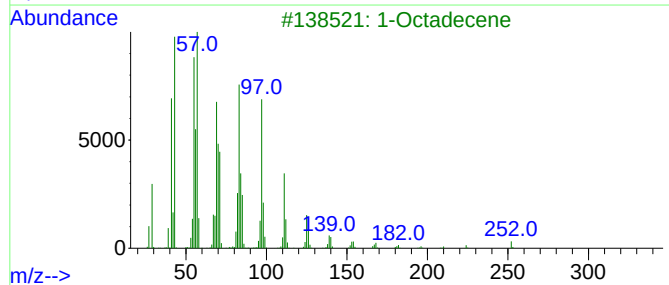
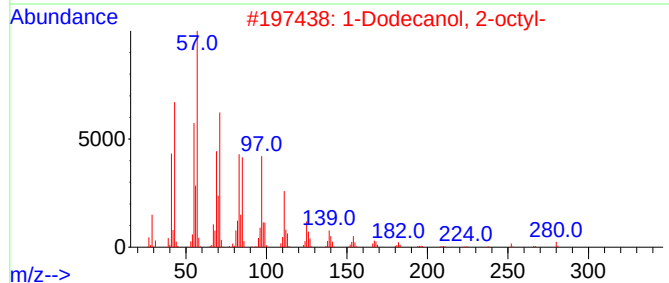
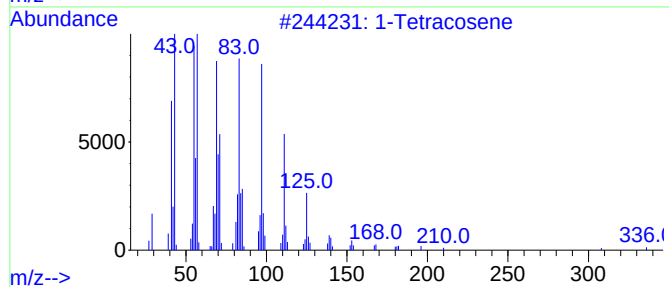
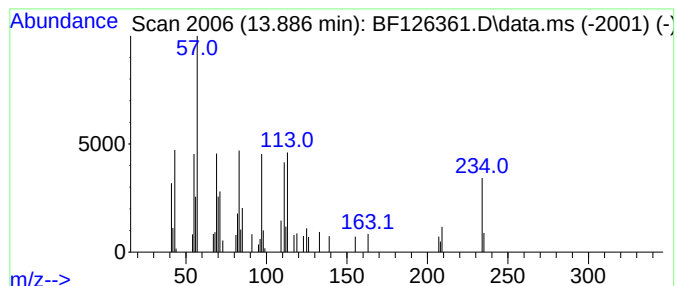
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.886 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.54 ng	78176	Chrysene-d12	13.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene		336	C24H48	010192-32-2	38
2	1-Dodecanol, 2-octyl-		298	C20H42O	005333-42-6	35
3	1-Octadecene		252	C18H36	000112-88-9	30
4	1-Hexacosene		364	C26H52	018835-33-1	27
5	Butyl eicosyl ether		354	C24H50O	1000406-40-7	27



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.381	3.9	ng	125152	1	6.810	639900	20.0
2-Pentanone, 4-...	5.004	5.0	ng	159854	1	6.810	639900	20.0
unknown13.886	13.886	2.5	ng	78176	5	13.968	615834	20.0