

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
 Data File : BF095731.D
 Acq On : 7 Jun 2017 2:55
 Operator : SJ/MA
 Sample : I3482-04 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-01-060517-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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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	4.569	504	507	528	rBV	34426	82125	7.31%	0.783%
2	5.269	622	626	654	rBV	515202	989065	88.07%	9.425%
3	6.934	906	909	922	rBV	577801	928405	82.67%	8.847%
4	7.039	922	927	938	rVB	750997	1122994	100.00%	10.702%
5	7.381	981	985	1000	rBV	302679	386296	34.40%	3.681%
6	7.616	1021	1025	1042	rBV	601857	805681	71.74%	7.678%
7	8.292	1136	1140	1159	rBV	410910	561277	49.98%	5.349%
8	9.416	1326	1331	1345	rBV	384951	494444	44.03%	4.712%
9	11.192	1628	1633	1646	rBV	909361	1022349	91.04%	9.742%
10	11.886	1747	1751	1758	rBV	82834	95378	8.49%	0.909%
11	12.239	1806	1811	1816	rBV2	364827	460447	41.00%	4.388%
12	12.286	1816	1819	1823	rVB3	10646	14865	1.32%	0.142%
13	13.098	1953	1957	1961	rBV	12497	14358	1.28%	0.137%
14	13.527	2026	2030	2038	rBV	349510	459030	40.88%	4.374%
15	13.868	2083	2088	2099	rBV2	13185	22290	1.98%	0.212%
16	14.627	2213	2217	2221	rVV2	325107	400946	35.70%	3.821%
17	14.668	2221	2224	2231	rVB	40943	58669	5.22%	0.559%
18	14.763	2236	2240	2246	rVB	13491	18593	1.66%	0.177%
19	15.439	2351	2355	2358	rVB	12079	13488	1.20%	0.129%
20	15.480	2358	2362	2368	rVB	14383	18609	1.66%	0.177%
21	15.551	2368	2374	2376	rBV3	8736	12013	1.07%	0.114%
22	15.586	2376	2380	2384	rVV2	18868	29752	2.65%	0.284%
23	15.645	2385	2390	2400	rVB3	35238	55592	4.95%	0.530%
24	16.245	2488	2492	2495	rBV2	16994	20446	1.82%	0.195%
25	16.286	2495	2499	2503	rVV4	9396	14082	1.25%	0.134%
26	16.368	2509	2513	2518	rVB4	11579	16933	1.51%	0.161%
27	16.445	2521	2526	2531	rBV	138204	163791	14.59%	1.561%
28	16.745	2572	2577	2585	rBV	164198	195001	17.36%	1.858%
29	16.939	2608	2610	2614	rBV3	8925	11285	1.00%	0.108%
30	16.998	2616	2620	2627	rVB	686647	768420	68.43%	7.323%
31	17.080	2627	2634	2637	rBV7	14820	28629	2.55%	0.273%
32	17.192	2647	2653	2654	rBV5	13534	18549	1.65%	0.177%
33	17.215	2655	2657	2663	rVB2	22434	30642	2.73%	0.292%
34	17.304	2669	2672	2677	rVB2	14784	18281	1.63%	0.174%

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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

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35	17.356	2677	2681	2687	rBV2	19746	40010	3.56%	0.381%
36	17.415	2688	2691	2697	rVB8	9437	11740	1.05%	0.112%
37	17.468	2697	2700	2703	rBV	18837	20297	1.81%	0.193%
38	17.856	2763	2766	2771	rBV6	19978	26372	2.35%	0.251%
39	18.051	2797	2799	2802	rVB2	17116	16608	1.48%	0.158%
40	18.086	2802	2805	2808	rBV4	10543	15504	1.38%	0.148%
41	18.262	2830	2835	2837	rBV4	45099	73521	6.55%	0.701%
42	18.345	2843	2849	2852	rBV2	378944	492056	43.82%	4.689%
43	18.380	2852	2855	2860	rVB	54856	75346	6.71%	0.718%
44	18.468	2868	2870	2875	rVB4	21863	27125	2.42%	0.258%
45	19.609	3062	3064	3068	rBV	43921	57486	5.12%	0.548%
46	20.015	3129	3133	3137	rBV	230862	284938	25.37%	2.715%

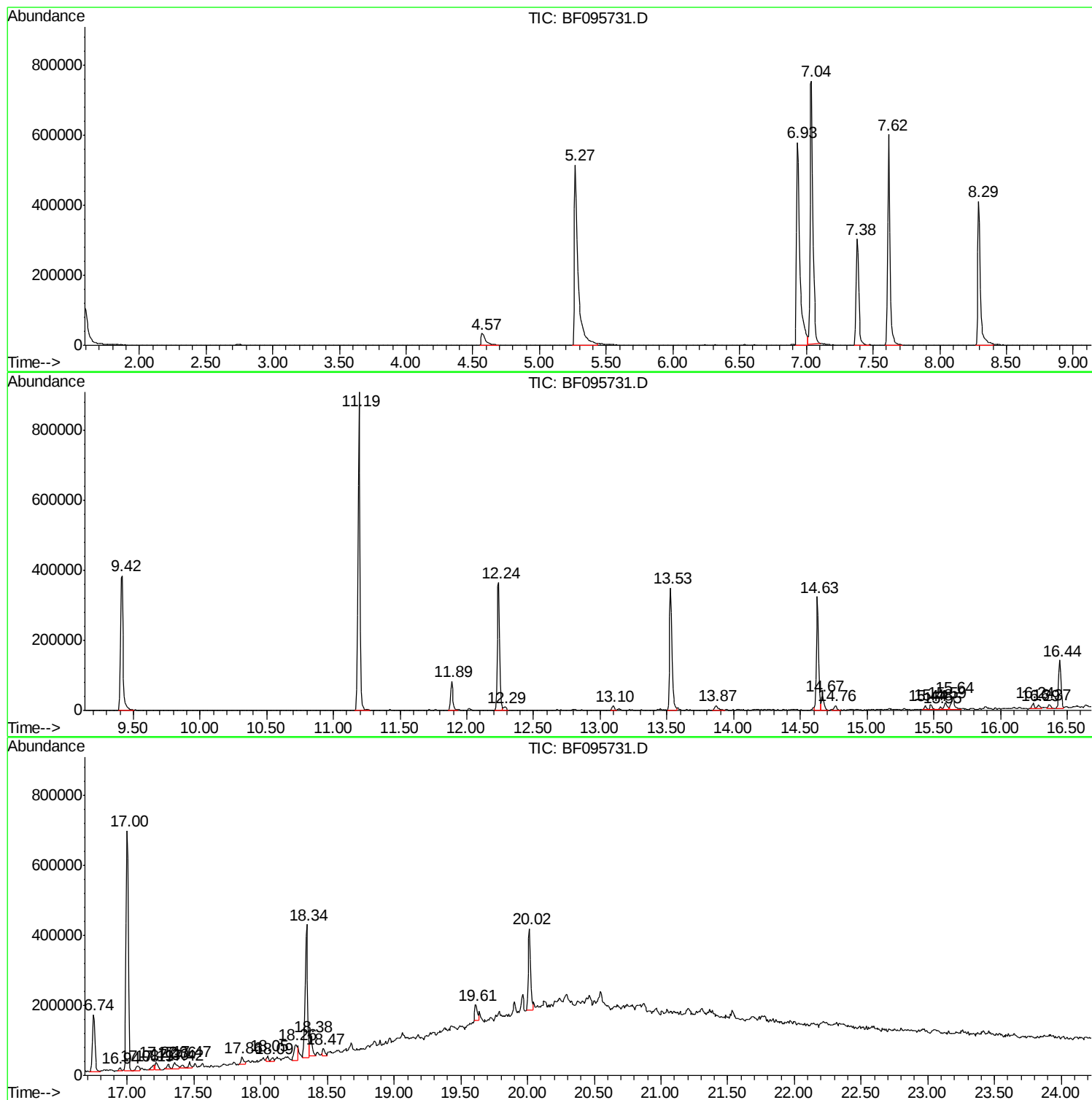
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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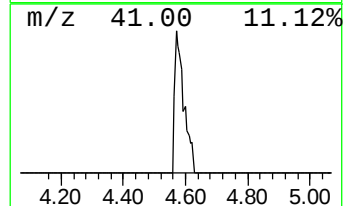
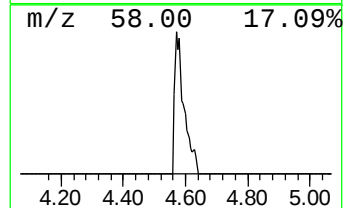
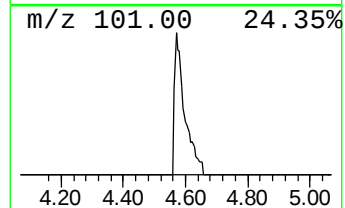
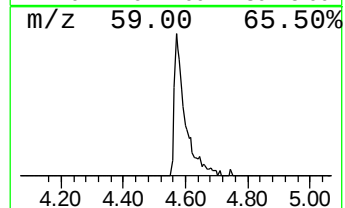
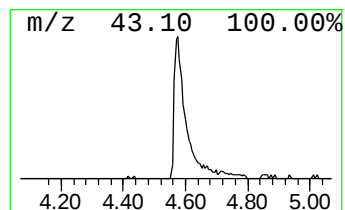
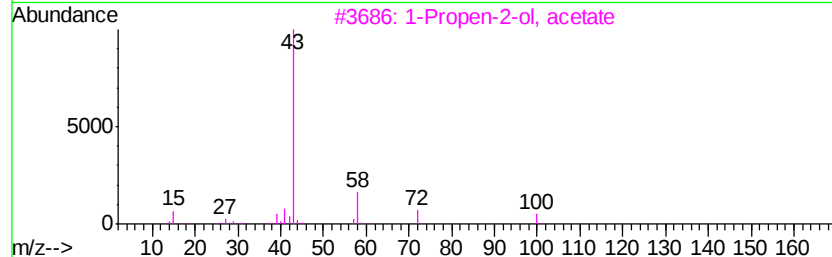
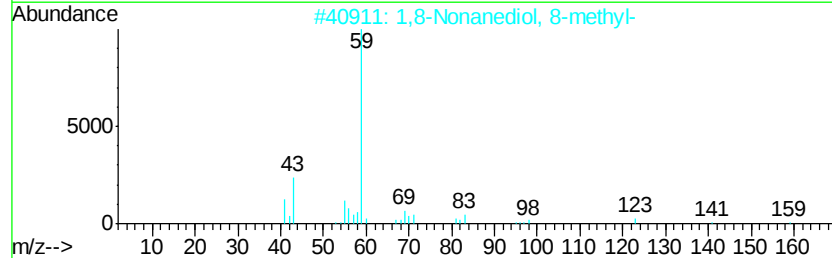
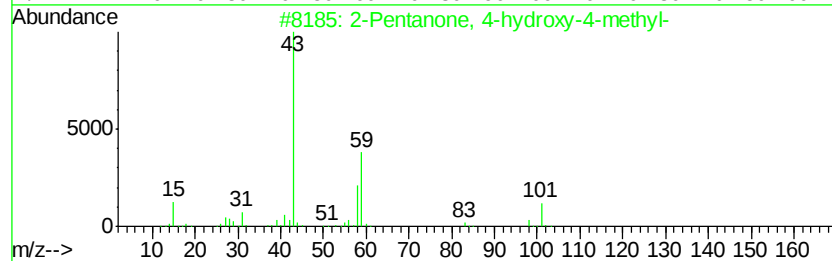
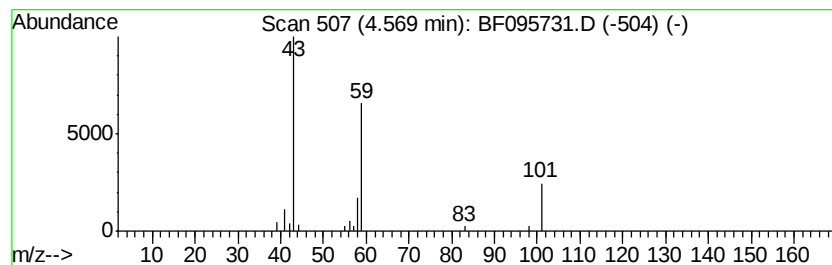
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	4.25 ng	82125	1,4-Dichlorobenzene-d4	7.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			3-Hexanol	102	C6H14O	000623-37-0	9
5			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9



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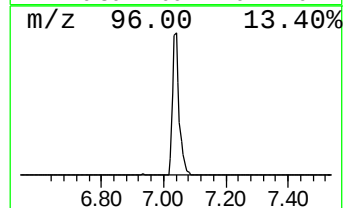
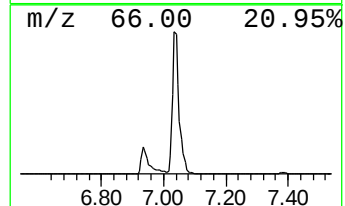
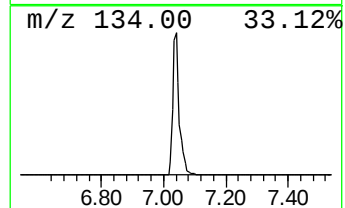
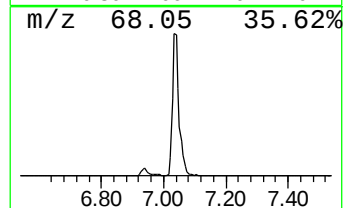
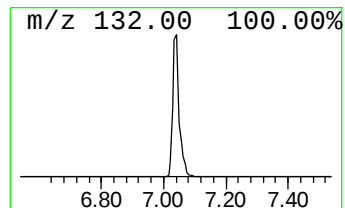
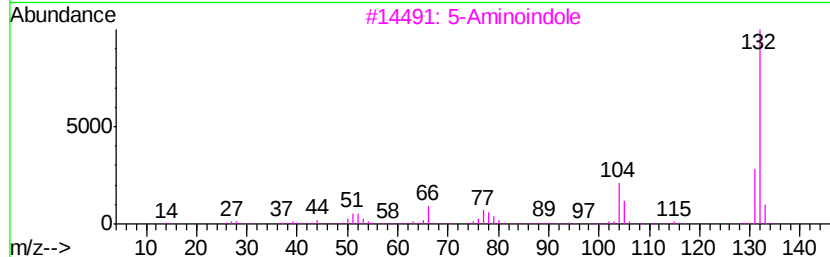
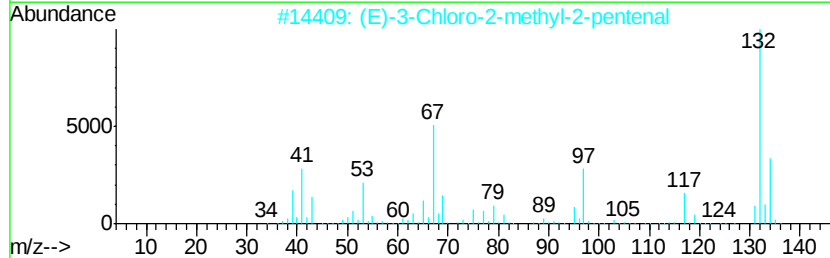
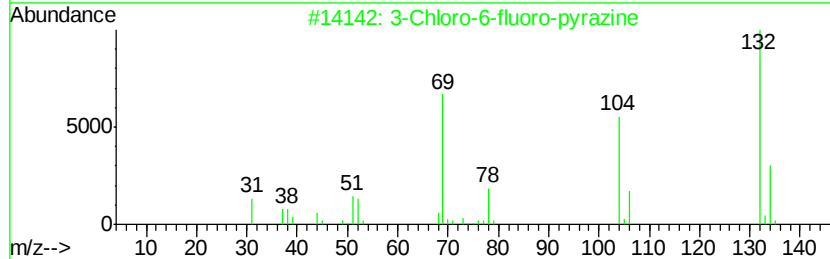
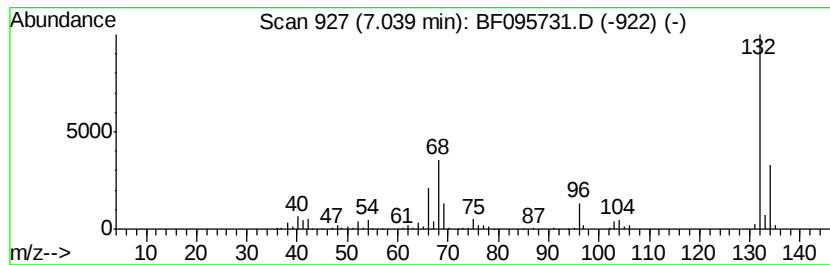
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	58.14 ng	1122990	1,4-Dichlorobenzene-d4	7.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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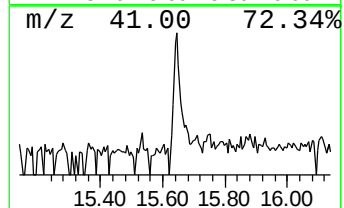
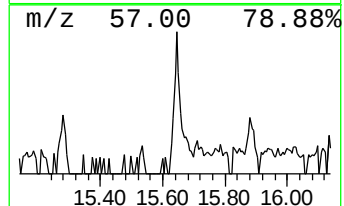
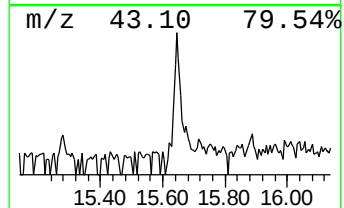
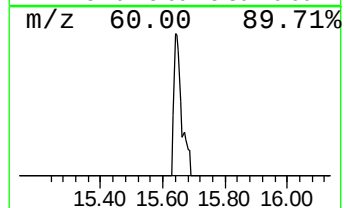
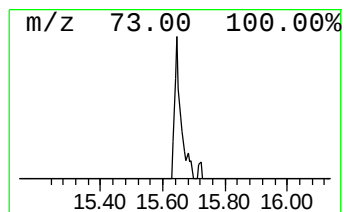
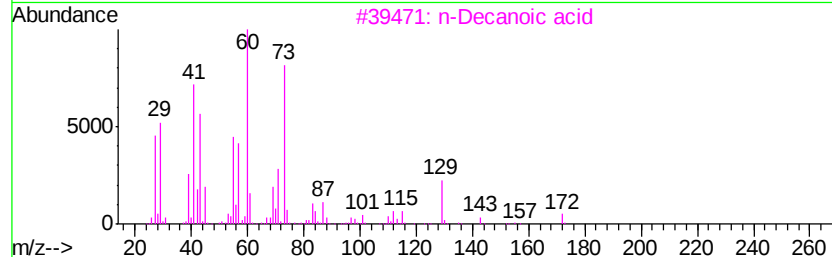
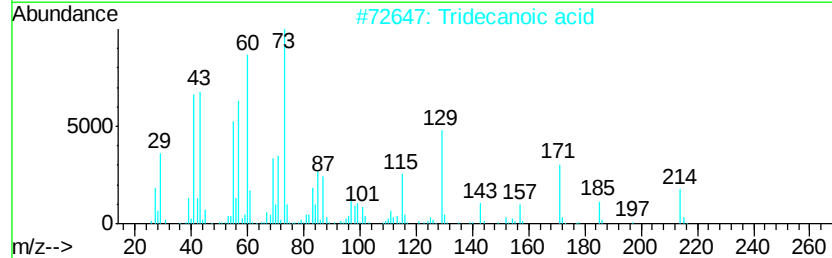
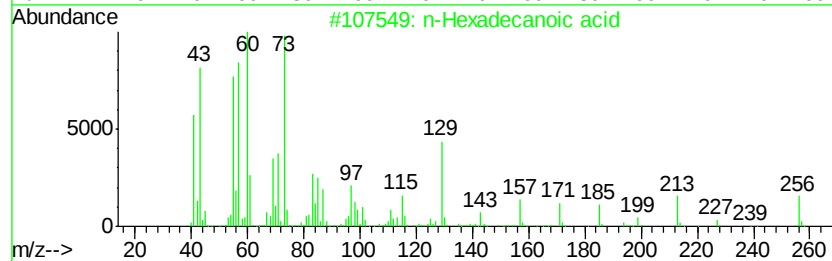
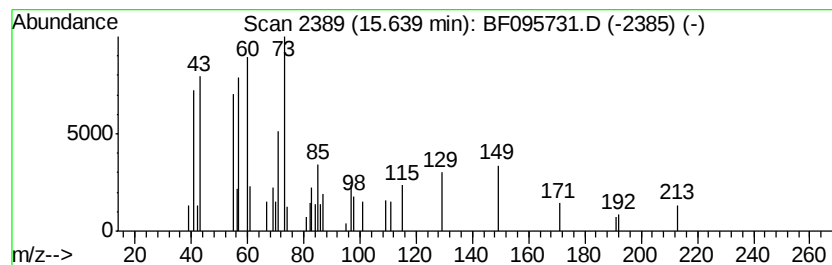
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.77 ng	55592	Phenanthrene-d10	14.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2		Tridecanoic acid	214	C13H26O2	000638-53-9	49
3		n-Decanoic acid	172	C10H20O2	000334-48-5	43
4		.beta.-D-Glucopyranoside, methyl...	334	C17H34O6	1000157-24-8	27
5		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	25



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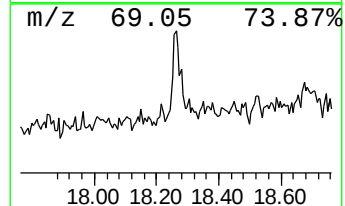
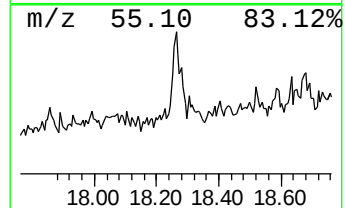
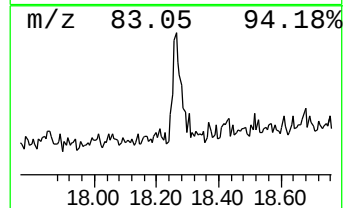
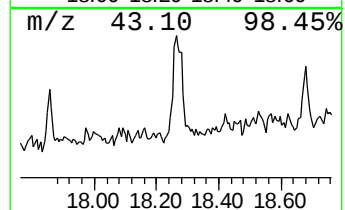
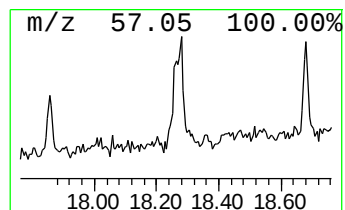
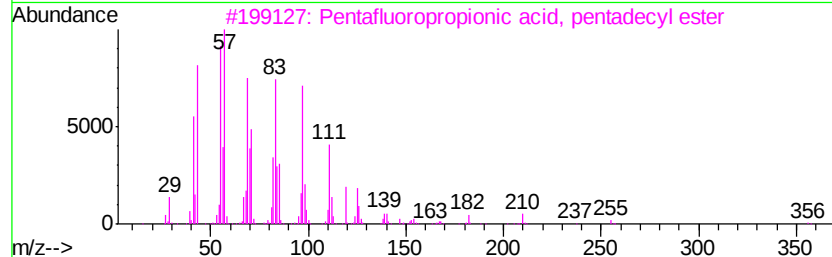
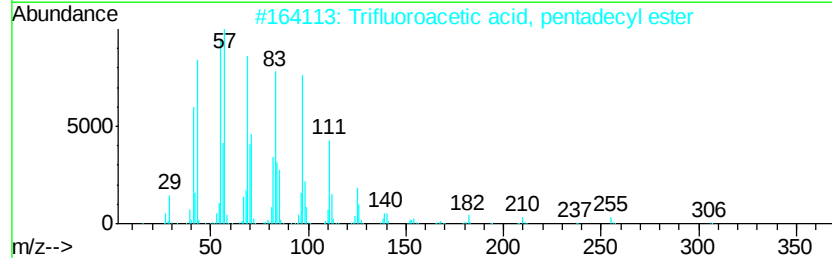
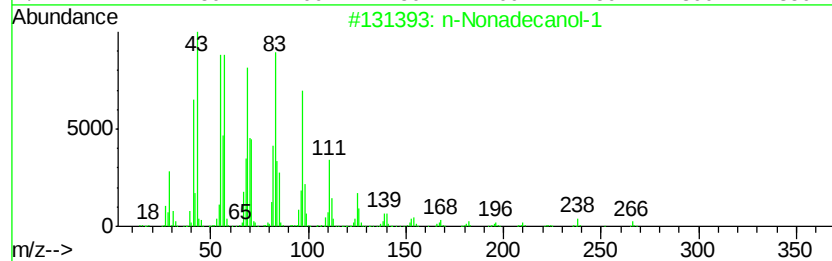
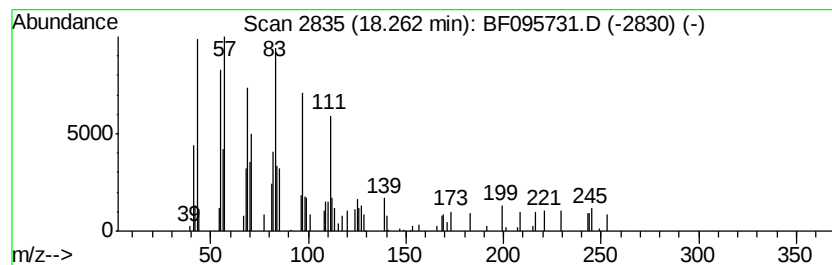
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.99 ng	73521	Chrysene-d12	18.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1		284	C19H40O	001454-84-8	93
2	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	93
3	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	93
4	1-Pentadecanethiol		244	C15H32S	025276-70-4	90
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	81



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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
2-Pentanone, 4-hy...	4.57	4.3	ng	82125	1	7.38	386296	20.0
unknown7.04	7.04	58.1	ng	1122990	1	7.38	386296	20.0
n-Hexadecanoic acid	15.64	2.8	ng	55592	4	14.63	400946	20.0
n-Nonadecanol-1	18.26	3.0	ng	73521	5	18.34	492056	20.0