

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061317\
 Data File : BF095900.D
 Acq On : 13 Jun 2017 18:34
 Operator : SJ/MA
 Sample : I3614-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-6

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	4.557	500	505	510	rBV2	9946	19946	1.09%	0.160%
2	5.257	620	624	646	rBV	134433	439202	23.91%	3.522%
3	6.934	906	909	918	rBV	97095	239432	13.04%	1.920%
4	7.004	918	921	943	rVB	598622	1220255	66.44%	9.786%
5	7.351	976	980	996	rVB	276975	388700	21.16%	3.117%
6	7.587	1015	1020	1038	rBV	604558	885856	48.23%	7.104%
7	8.269	1132	1136	1155	rBV	470956	776528	42.28%	6.227%
8	8.863	1231	1237	1245	rBV3	9711	20395	1.11%	0.164%
9	9.380	1321	1325	1343	rBV	365067	589806	32.11%	4.730%
10	10.163	1454	1458	1463	rBV5	12154	19912	1.08%	0.160%
11	10.710	1546	1551	1555	rVB4	18434	27815	1.51%	0.223%
12	10.827	1568	1571	1577	rVB7	18130	30226	1.65%	0.242%
13	10.886	1577	1581	1585	rBV6	12788	22949	1.25%	0.184%
14	10.945	1585	1591	1595	rVV7	11038	23624	1.29%	0.189%
15	11.033	1602	1606	1611	rBV6	16650	35349	1.92%	0.283%
16	11.157	1622	1627	1638	rBV	1381979	1836592	100.00%	14.728%
17	11.392	1662	1667	1669	rBV4	11354	20250	1.10%	0.162%
18	11.545	1689	1693	1700	rVB7	16214	31623	1.72%	0.254%
19	11.657	1708	1712	1716	rBV3	25427	34139	1.86%	0.274%
20	11.751	1723	1728	1730	rBV4	14037	23024	1.25%	0.185%
21	11.863	1742	1747	1763	rVB	84068	159296	8.67%	1.277%
22	12.133	1790	1793	1799	rVB7	16319	28228	1.54%	0.226%
23	12.204	1800	1805	1812	rBV2	462235	631743	34.40%	5.066%
24	12.339	1820	1828	1832	rBV10	13607	32599	1.77%	0.261%
25	12.486	1849	1853	1859	rVB8	13806	24921	1.36%	0.200%
26	12.751	1893	1898	1901	rVB7	10708	19767	1.08%	0.159%
27	12.921	1924	1927	1937	rVB10	21240	47629	2.59%	0.382%
28	13.221	1972	1978	1982	rBV8	24168	42906	2.34%	0.344%
29	13.268	1982	1986	1991	rVB7	17167	28751	1.57%	0.231%
30	13.498	2020	2025	2038	rBV	797870	1125571	61.29%	9.026%
31	14.292	2156	2160	2167	rVB9	13101	21825	1.19%	0.175%
32	14.598	2207	2212	2222	rBV	439021	585146	31.86%	4.693%
33	15.621	2379	2386	2393	rBV2	110982	168960	9.20%	1.355%
34	16.721	2569	2573	2583	rBV	105002	147259	8.02%	1.181%

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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	16.974	2610	2616	2627	rVB	1552879	1829266	99.60%	14.670%
36	17.780	2749	2753	2758	rBV	47138	59474	3.24%	0.477%
37	18.233	2826	2830	2834	rBV3	28994	39819	2.17%	0.319%
38	18.315	2840	2844	2854	rBV	325223	451409	24.58%	3.620%
39	19.992	3125	3129	3141	rBV	220411	339462	18.48%	2.722%

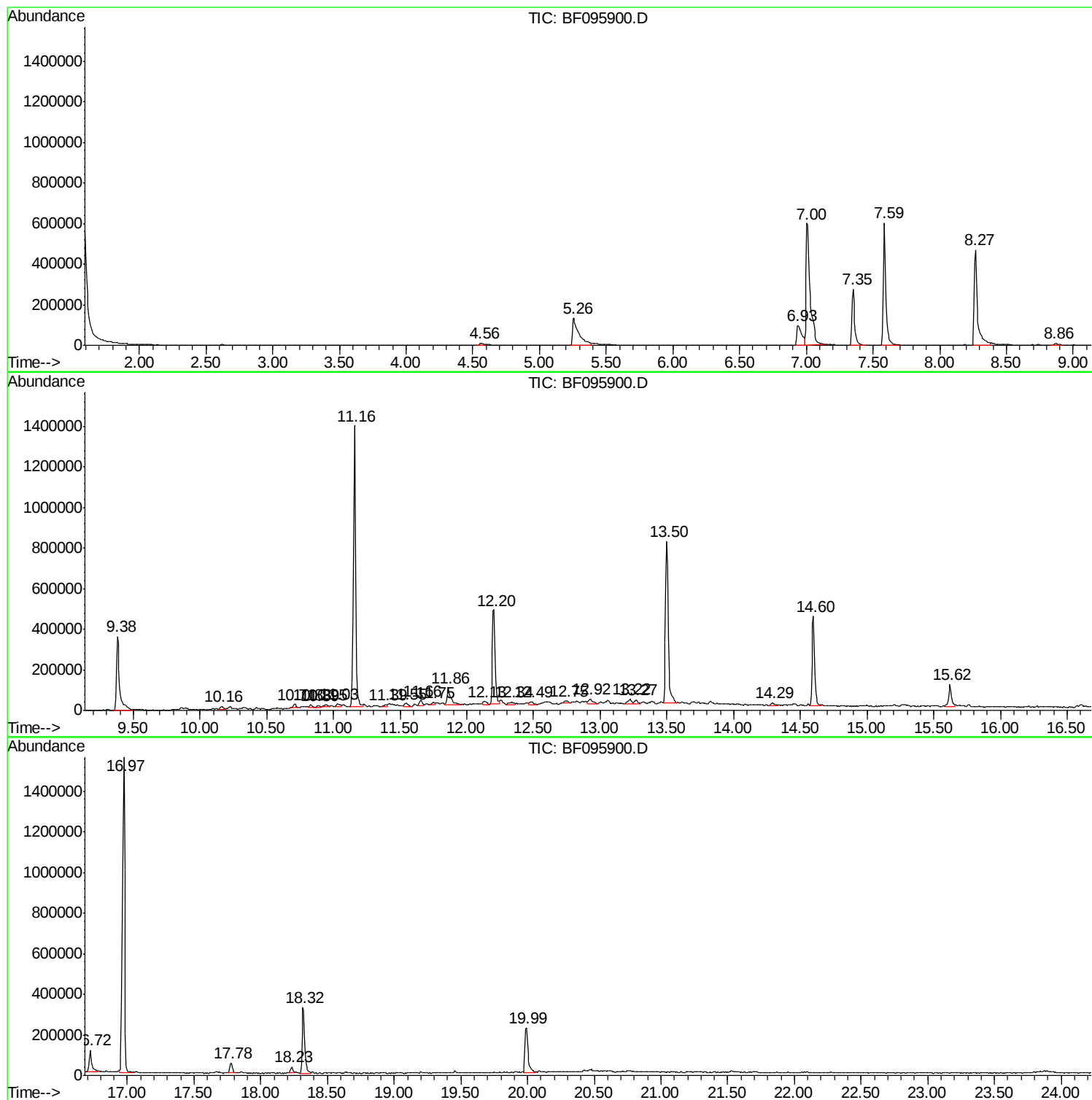
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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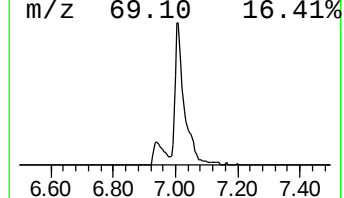
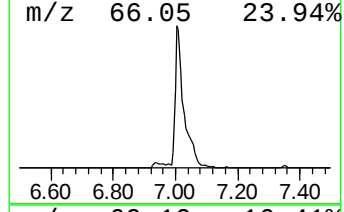
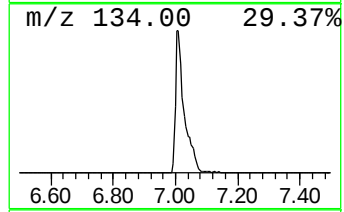
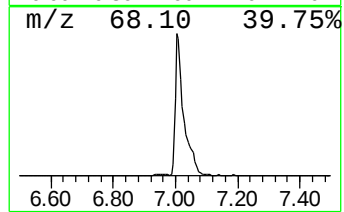
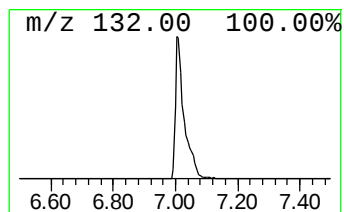
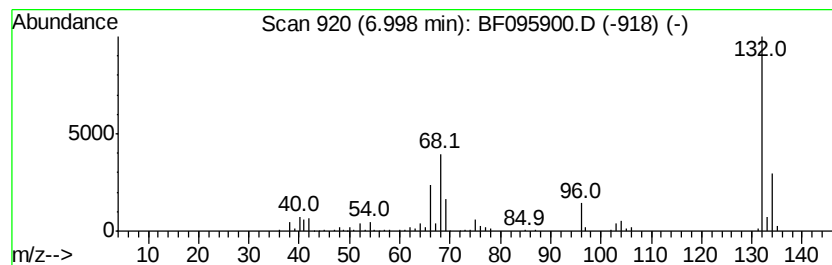
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	62.79 ng	1220260	1,4-Dichlorobenzene-d4	7.35

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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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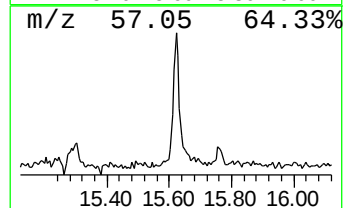
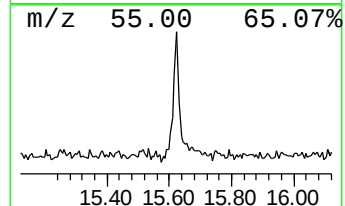
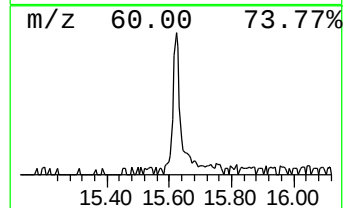
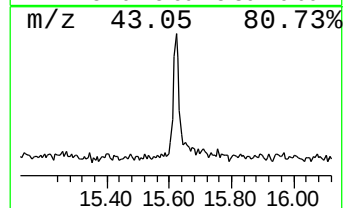
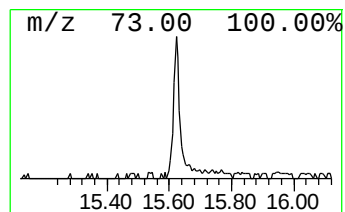
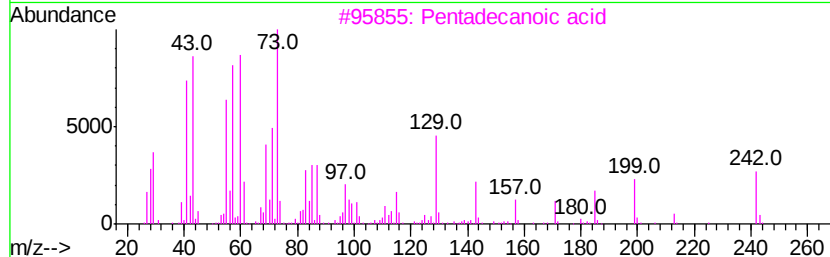
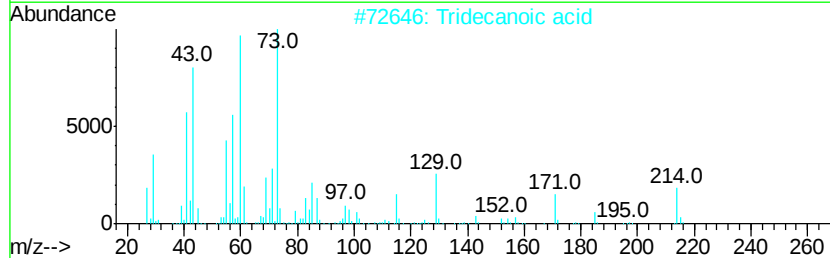
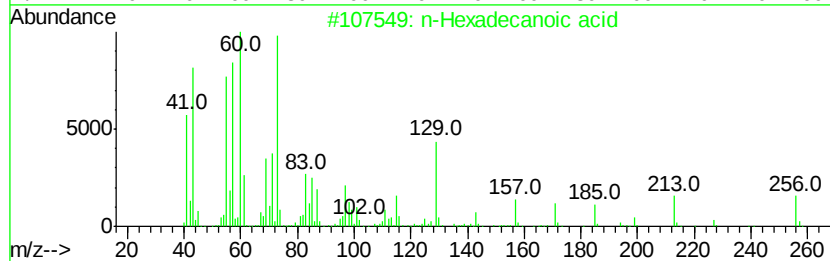
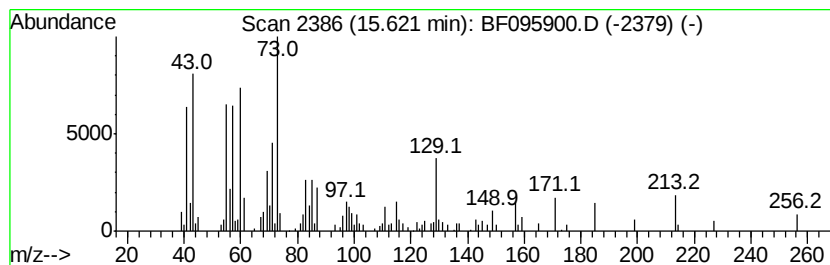
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.62	5.77 ng	168960	Phenanthrene-d10	14.60	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	20



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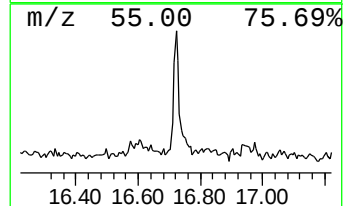
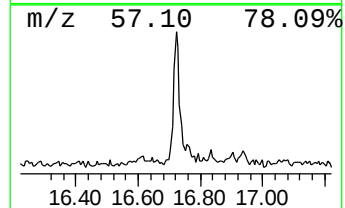
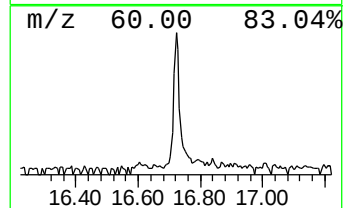
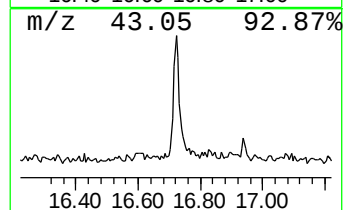
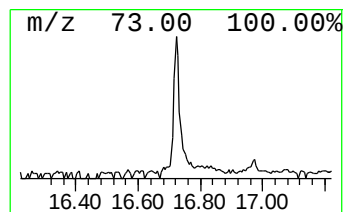
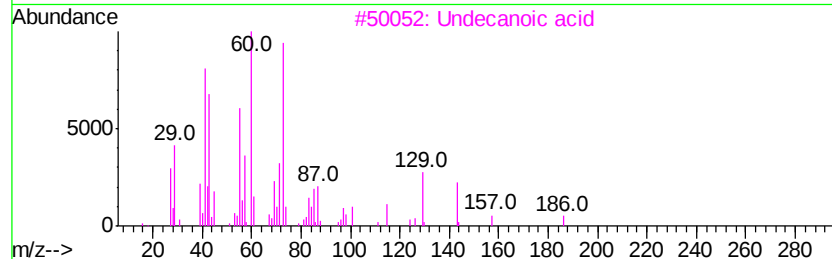
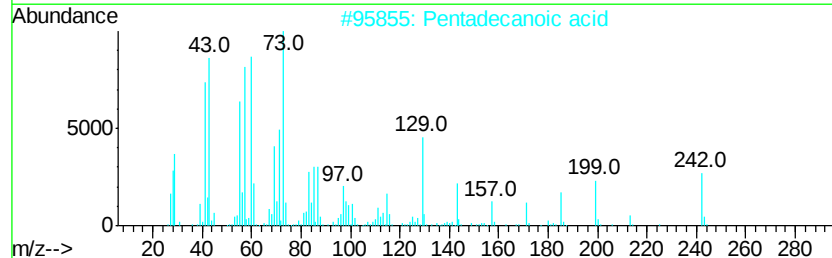
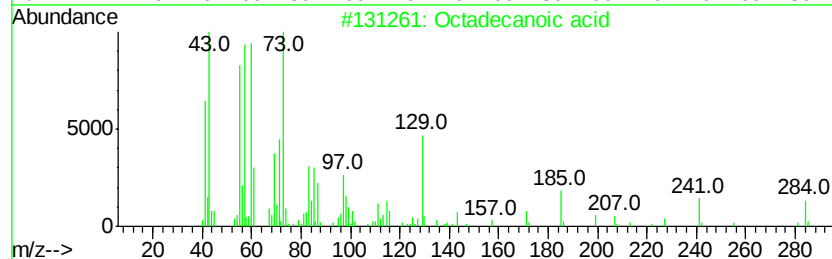
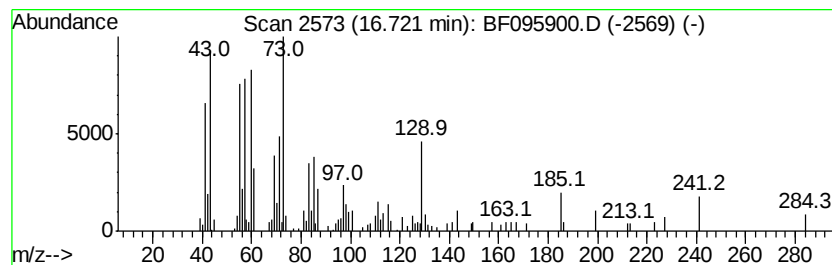
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.72	6.52 ng	147259	Chrysene-d12		18.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Pentadecane	212	C15H32	000629-62-9	53
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25



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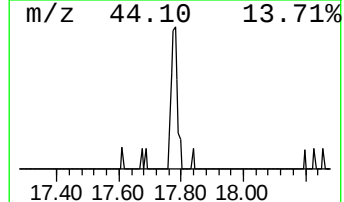
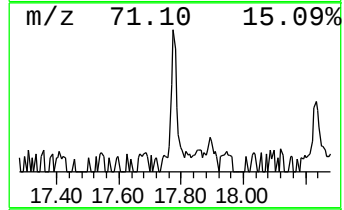
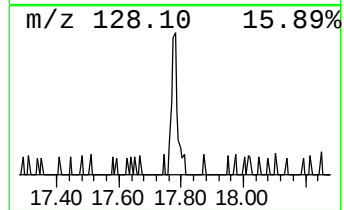
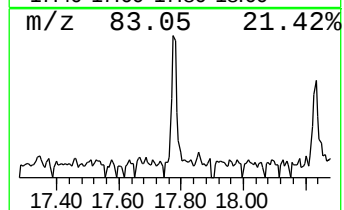
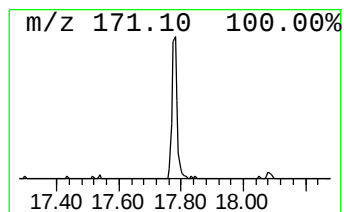
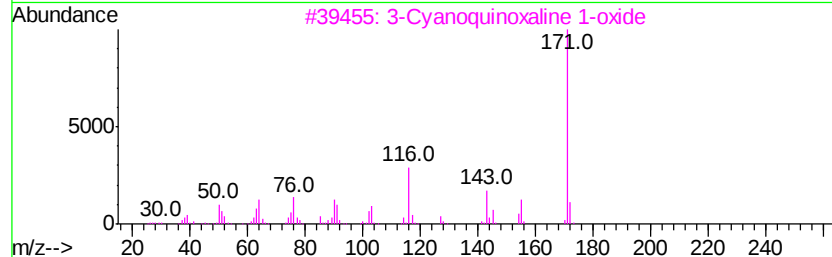
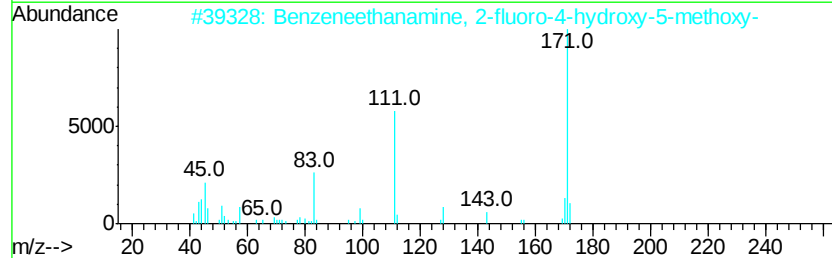
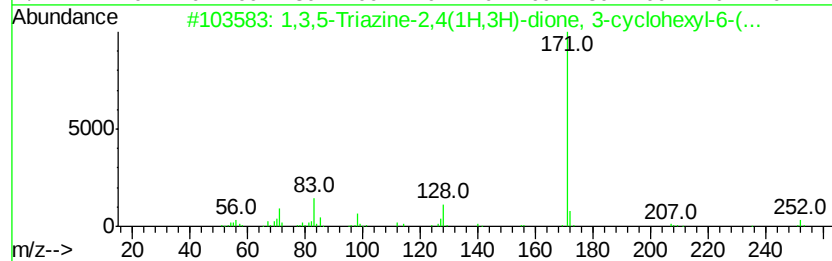
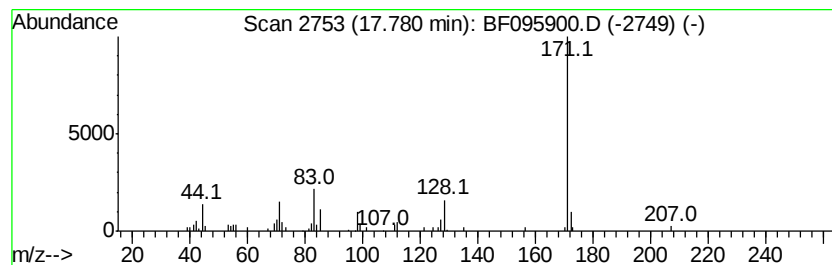
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.78	2.64 ng	59474	Chrysene-d12	18.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	90
2		Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	64
3		3-Cyanoquinoxaline 1-oxide	171	C9H5N3O	053688-02-1	50
4		Pyridine, 4-phenyl-, 1-oxide	171	C11H9NO	001131-61-9	47
5		4-Pyridinol, 2-phenyl-	171	C11H9NO	1000253-54-5	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.00	7.00	62.8	ng	1220260	1	7.35	388700	20.0
n-Hexadecanoic acid	15.62	5.8	ng	168960	4	14.60	585146	20.0
Octadecanoic acid	16.72	6.5	ng	147259	5	18.32	451409	20.0
1,3,5-Triazine-2,...	17.78	2.6	ng	59474	5	18.32	451409	20.0