

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
 Data File : BF094954.D
 Acq On : 6 May 2017 11:20
 Operator : SJ/MA
 Sample : I2947-08
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-8.5-9.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	5.043	524	528	551	rBV	127744	265967	10.90%	1.251%
2	5.666	630	634	657	rBV	1448206	2209048	90.51%	10.390%
3	7.260	900	905	921	rBV	1569938	2231197	91.42%	10.495%
4	7.384	921	926	939	rVB	1829855	2440612	100.00%	11.479%
5	7.719	979	983	999	rVB	444052	535075	21.92%	2.517%
6	7.960	1019	1024	1038	rBV	1563899	1822294	74.67%	8.571%
7	8.619	1131	1136	1155	rBV	1041084	1385418	56.77%	6.516%
8	9.742	1322	1327	1343	rBV	523898	731274	29.96%	3.440%
9	11.513	1623	1628	1645	rBV	1893349	2377079	97.40%	11.181%
10	12.207	1741	1746	1758	rBV	238977	323514	13.26%	1.522%
11	12.571	1803	1808	1821	rBV2	622476	883071	36.18%	4.154%
12	13.413	1947	1951	1956	rBV	42183	49400	2.02%	0.232%
13	13.866	2023	2028	2043	rBV	1003493	1555350	63.73%	7.316%
14	14.189	2077	2083	2086	rBV	36638	45835	1.88%	0.216%
15	14.971	2211	2216	2230	rBV2	499310	742813	30.44%	3.494%
16	15.942	2376	2381	2393	rBV	57819	88799	3.64%	0.418%
17	17.295	2606	2611	2623	rBV	1784110	2128415	87.21%	10.011%
18	18.130	2747	2753	2757	rBV	40008	42738	1.75%	0.201%
19	18.548	2820	2824	2828	rBV	57914	58168	2.38%	0.274%
20	18.642	2835	2840	2855	rVB	466828	695520	28.50%	3.271%
21	18.948	2888	2892	2897	rVB	46730	45140	1.85%	0.212%
22	19.330	2954	2957	2962	rVB	25668	26340	1.08%	0.124%
23	20.306	3118	3123	3135	rBV	298013	439802	18.02%	2.069%
24	20.777	3195	3203	3216	rBV4	30031	82310	3.37%	0.387%
25	21.206	3269	3276	3283	rBV4	14346	28084	1.15%	0.132%
26	22.265	3450	3456	3465	rBV7	10204	27366	1.12%	0.129%

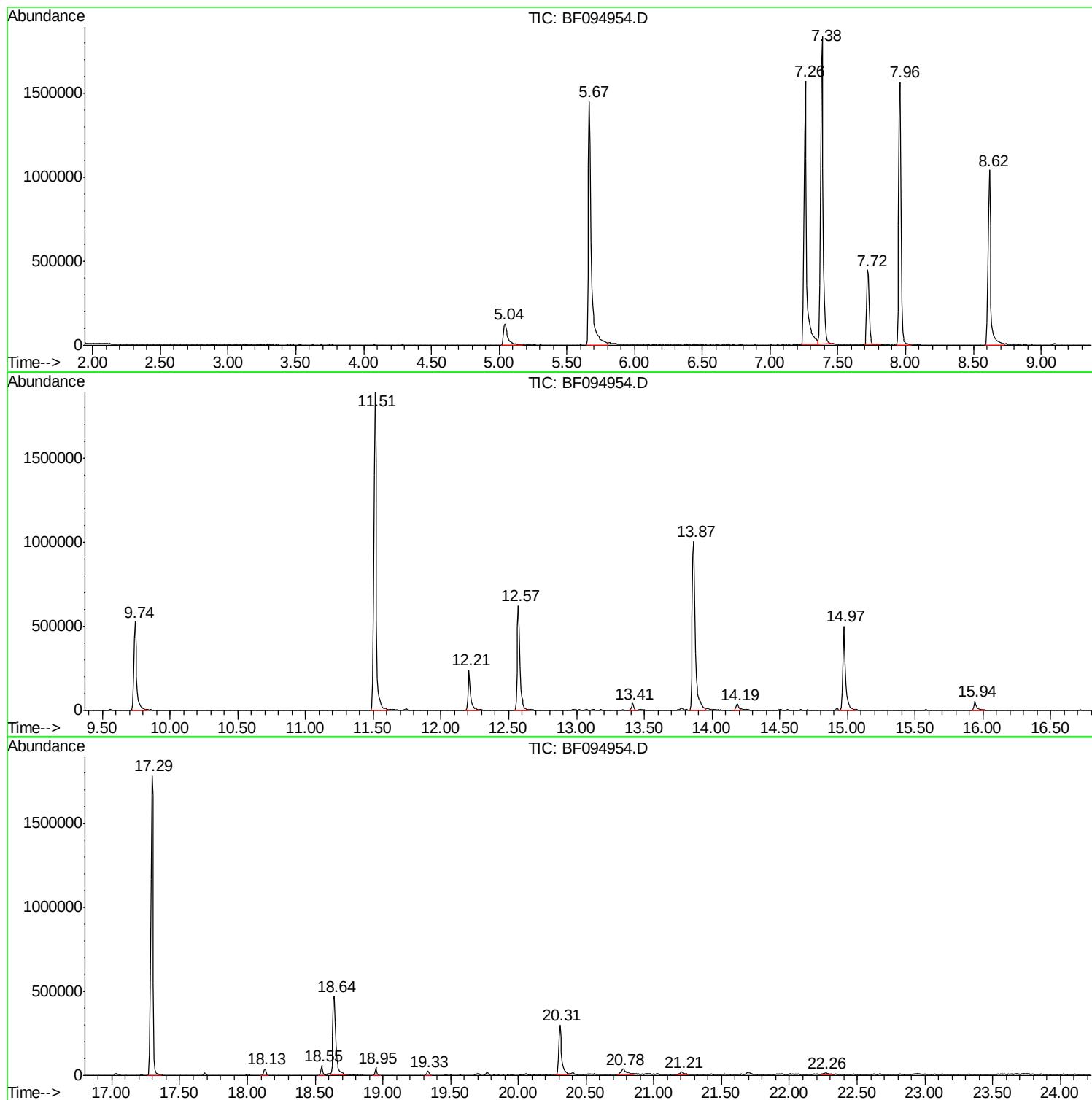
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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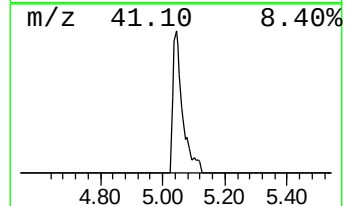
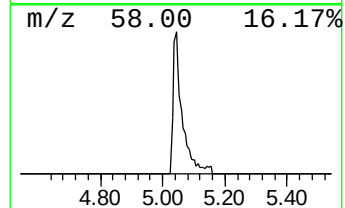
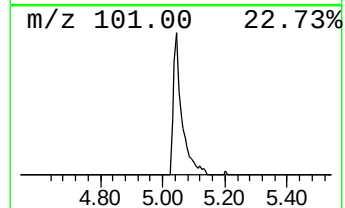
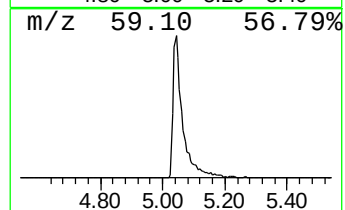
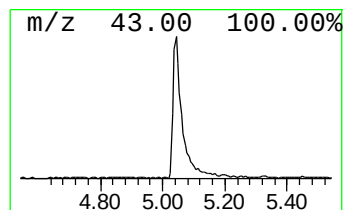
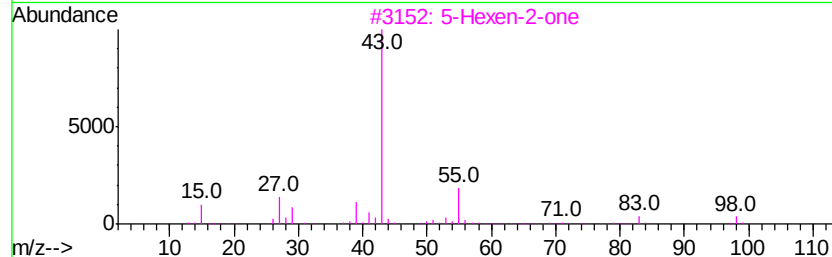
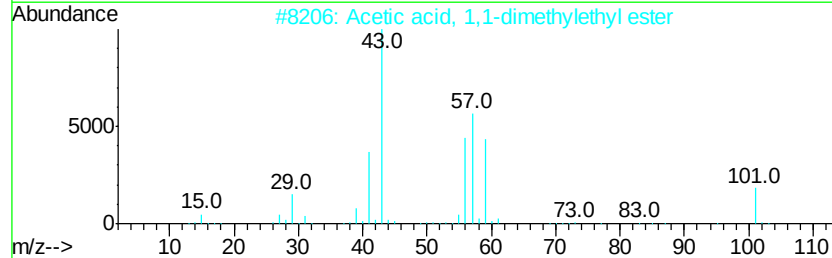
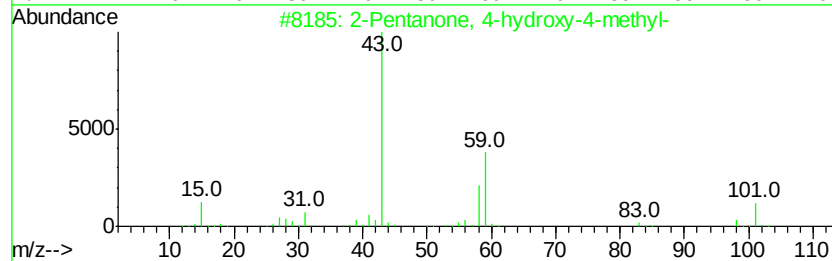
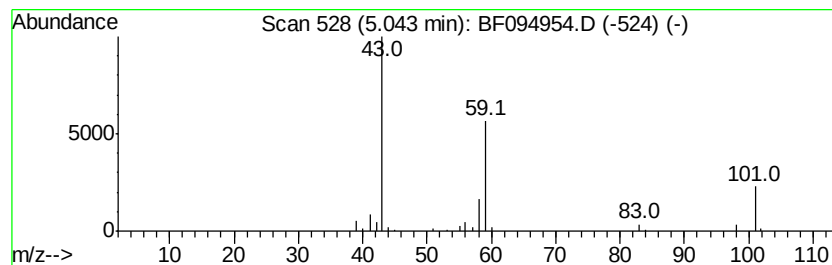
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.04	9.94 ng	265967	1,4-Dichlorobenzene-d4	7.72

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			5-Hexen-2-one	98	C6H10O	000109-49-9	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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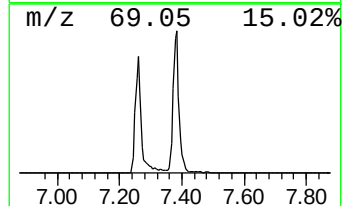
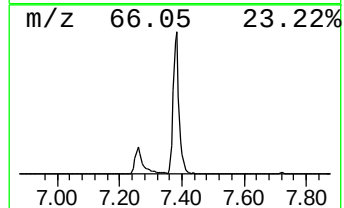
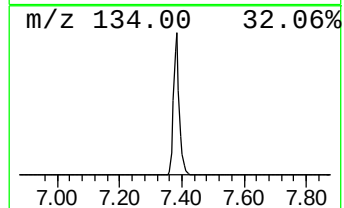
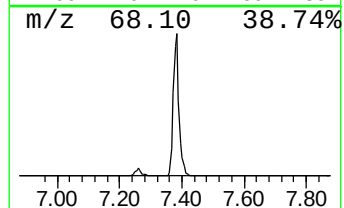
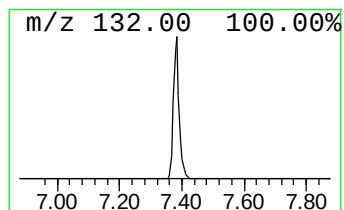
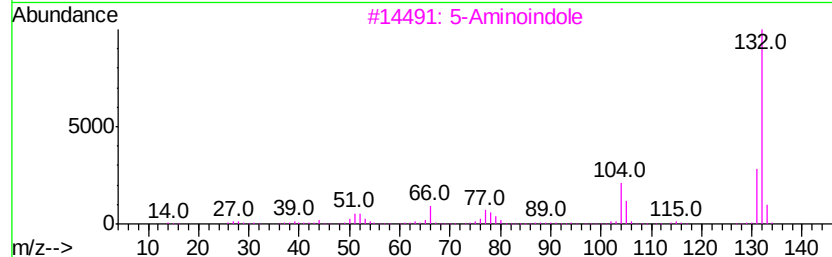
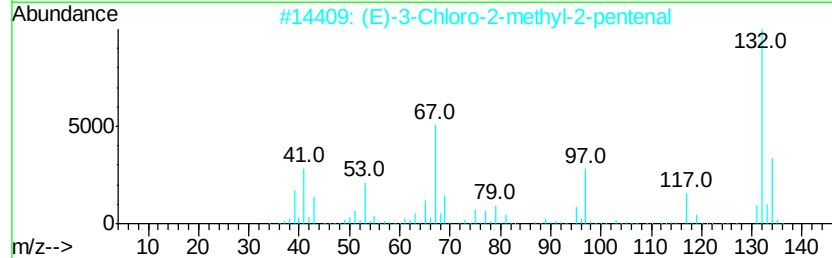
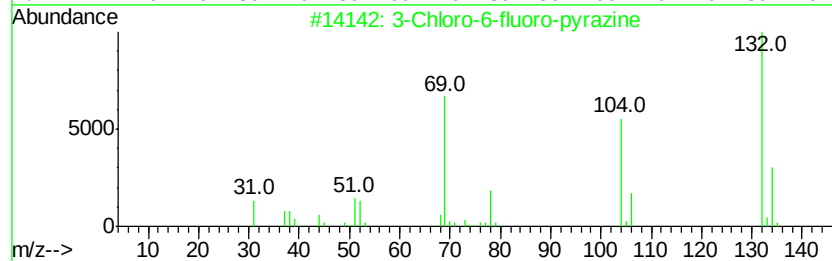
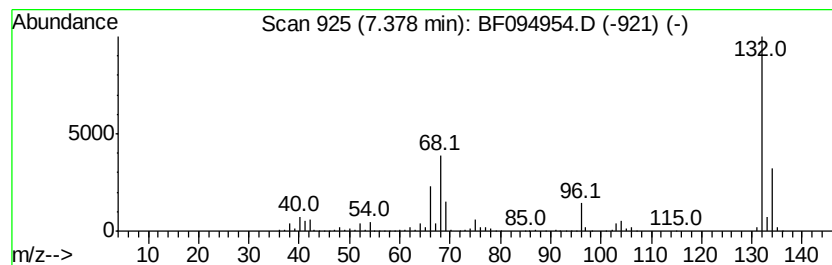
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	91.23 ng	2440610	1,4-Dichlorobenzene-d4	7.72

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		Xenon	132	Xe	007440-63-3	9



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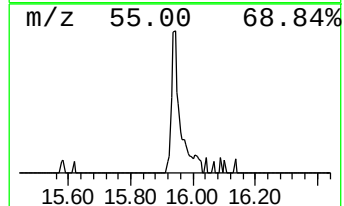
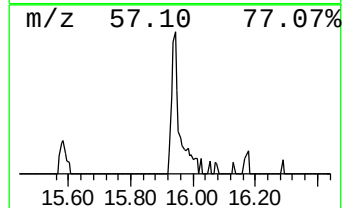
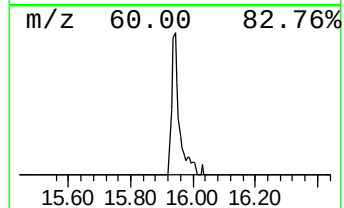
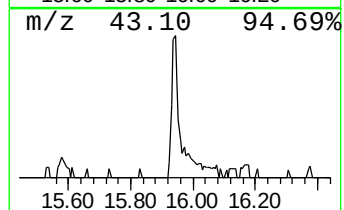
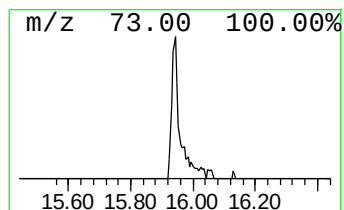
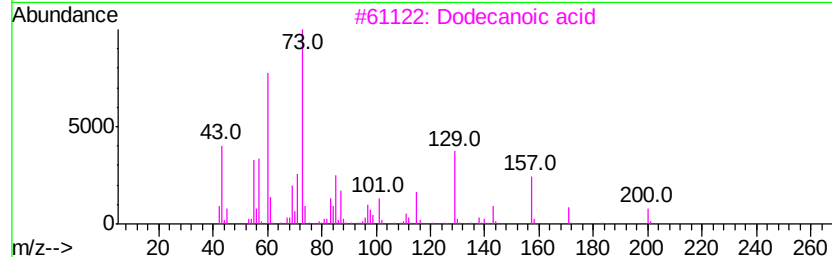
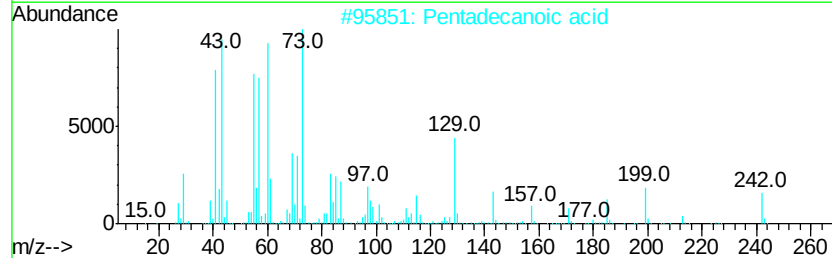
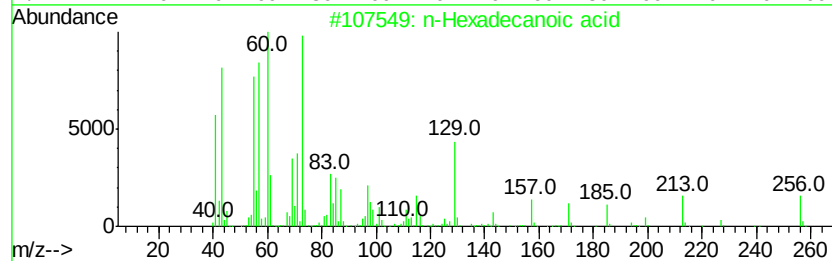
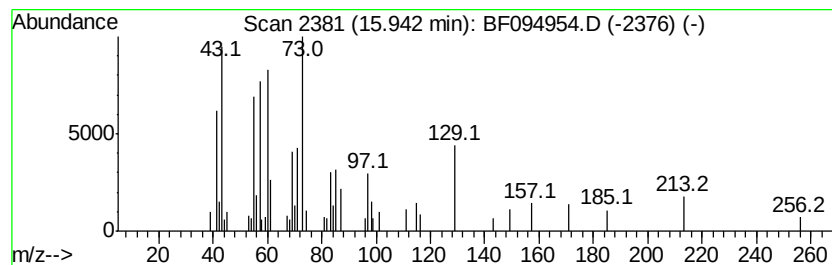
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.39 ng	88799	Phenanthrene-d10	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Isoamyl nitrite	117	C5H11NO2	000110-46-3	27
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14



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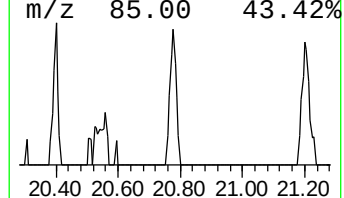
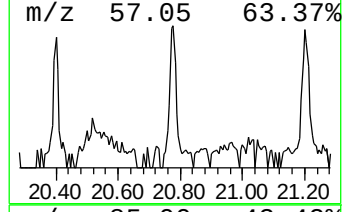
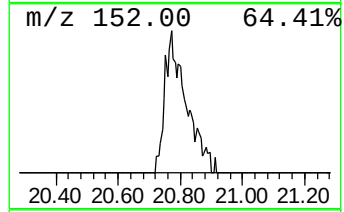
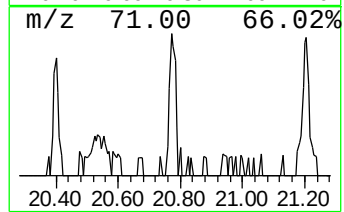
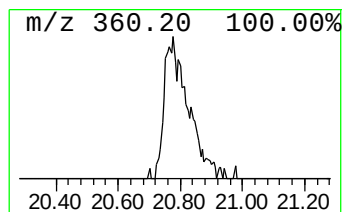
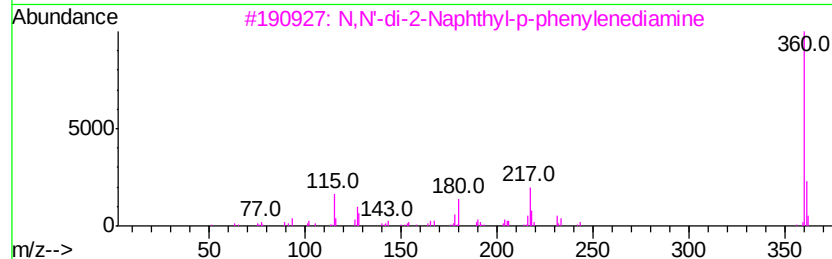
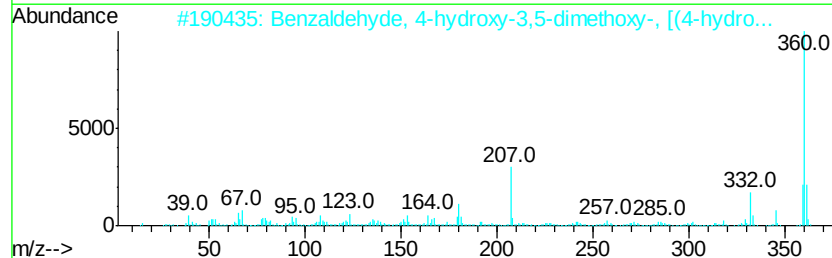
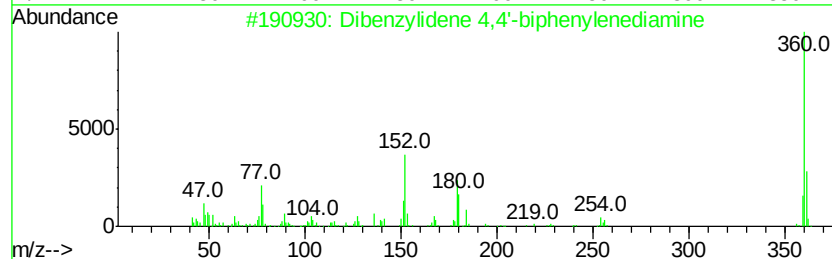
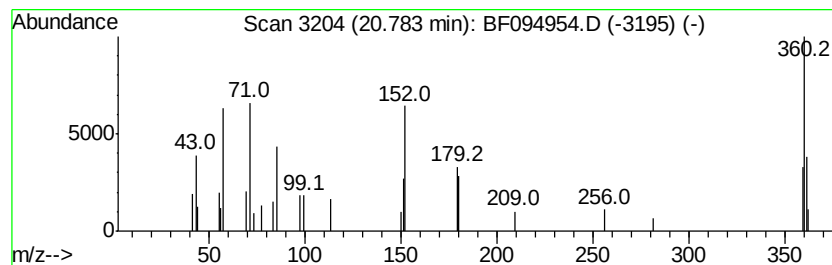
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	3.74 ng	82310	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	70
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	37
3		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	35
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	32
5		Octadecane	254	C18H38	000593-45-3	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	9.9	ng	265967	1	7.72	535075	20.0
unknown7.38	7.38	91.2	ng	2440610	1	7.72	535075	20.0
n-Hexadecanoic acid	15.94	2.4	ng	88799	4	14.97	742813	20.0
Dibenzylidene 4,4...	20.78	3.7	ng	82310	6	20.31	439802	20.0