

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
 Data File : BM018231.D
 Acq On : 16 Dec 2018 17:53
 Operator : JU/SJ
 Sample : J6377-16
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P001-SD006-0612-01

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_M\METHODS\8270-BM121518.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	4.693	301	307	313	rBV	80458	116423	2.72%	0.333%
2	5.128	375	381	392	rBV	2374073	3343277	78.11%	9.562%
3	6.698	641	648	666	rBV	2212069	3694067	86.31%	10.565%
4	7.040	698	706	723	rBV	2406031	3726911	87.08%	10.659%
5	7.492	777	783	793	rVB	485549	764076	17.85%	2.185%
6	7.810	830	837	847	rVB	1781114	2773838	64.81%	7.933%
7	8.657	973	981	1000	rBV	1236624	2132171	49.82%	6.098%
8	10.263	1247	1254	1273	rBV	526044	990585	23.14%	2.833%
9	12.763	1672	1679	1695	rBV	2865972	4279994	100.00%	12.240%
10	13.633	1821	1827	1839	rBV	119582	207769	4.85%	0.594%
11	14.157	1909	1916	1927	rBV2	749461	1178816	27.54%	3.371%
12	15.663	2165	2172	2187	rBV	1993335	2941277	68.72%	8.412%
13	16.915	2379	2385	2399	rBV2	782501	1230713	28.76%	3.520%
14	17.827	2535	2540	2550	rBV	98679	165981	3.88%	0.475%
15	19.127	2756	2761	2769	rBV6	35130	58944	1.38%	0.169%
16	19.568	2831	2836	2848	rBV	3251851	4161087	97.22%	11.900%
17	20.862	3052	3056	3064	rVB	193748	249211	5.82%	0.713%
18	21.139	3098	3103	3112	rBV	974318	1345630	31.44%	3.848%
19	21.721	3200	3202	3204	rBV2	63792	68197	1.59%	0.195%
20	21.750	3204	3207	3214	rVB5	117793	188599	4.41%	0.539%
21	23.297	3464	3470	3481	rBV	715688	1348461	31.51%	3.856%

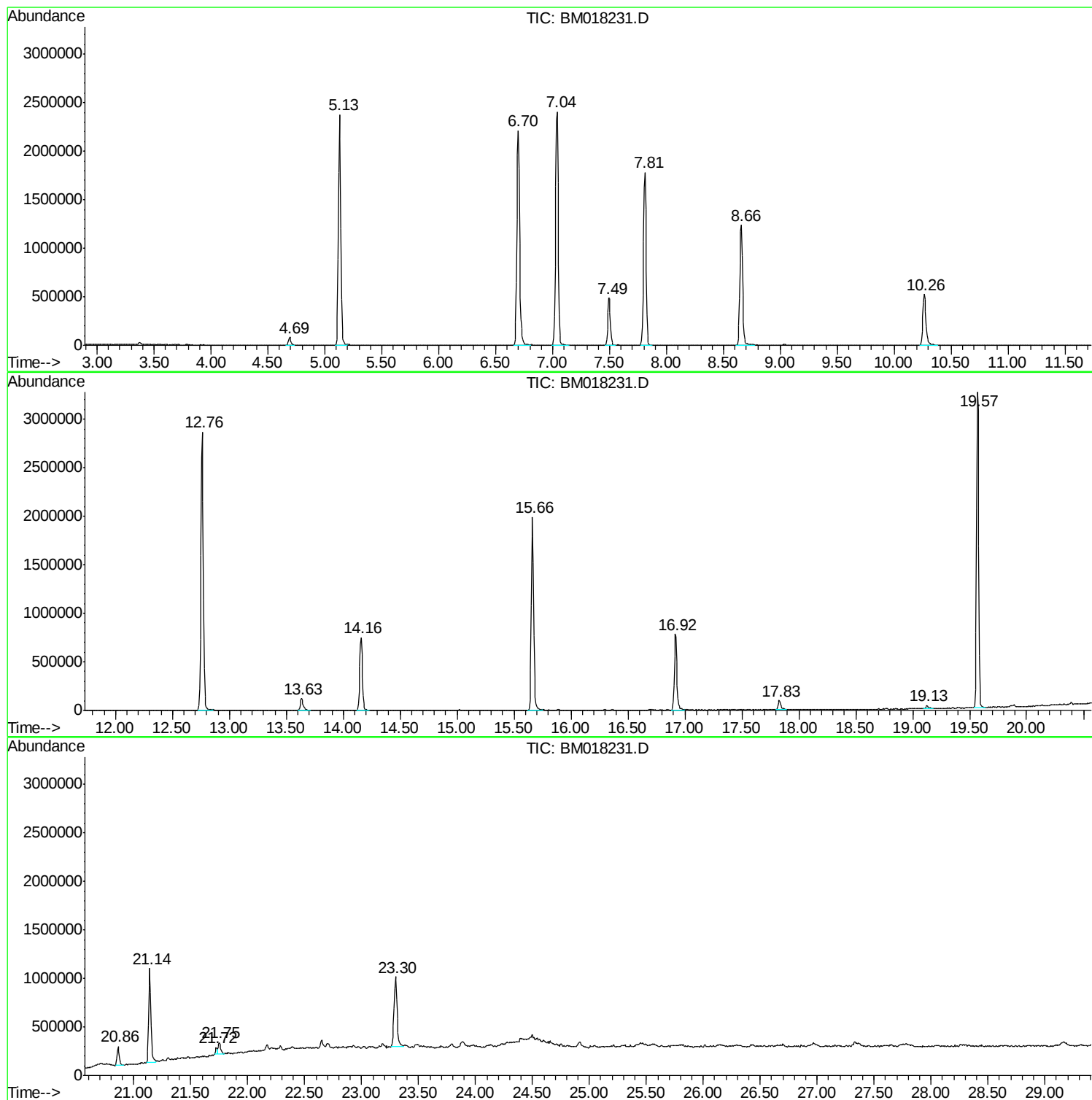
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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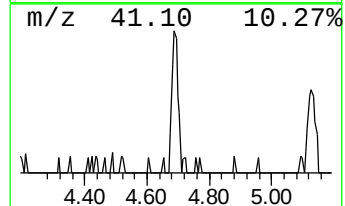
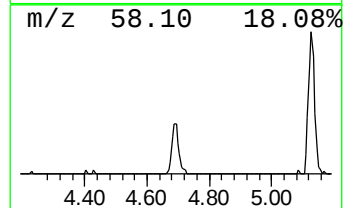
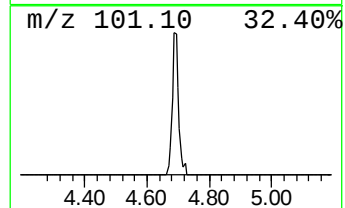
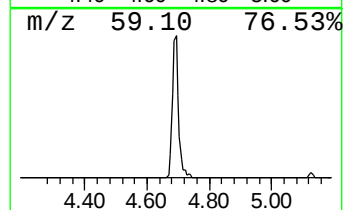
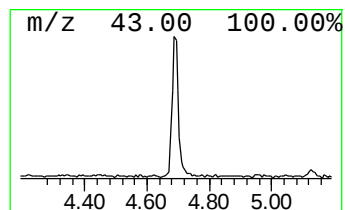
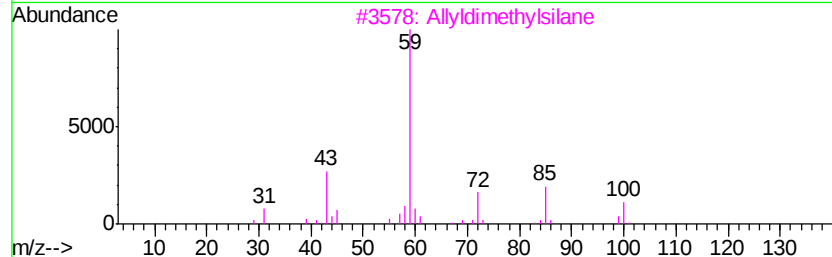
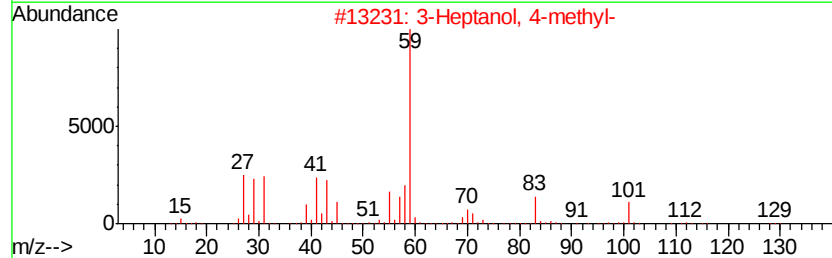
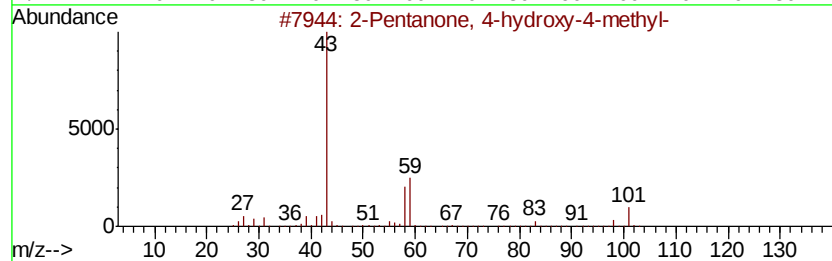
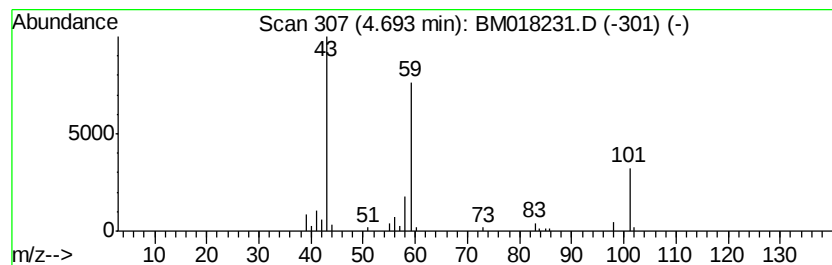
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	3.05 ng	116423	1,4-Dichlorobenzene-d4	7.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
3			Allyldimethylsilane	100	C5H12Si	003937-30-2	28
4			Pentanal, oxime	101	C5H11NO	000628-79-5	28
5			Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	25



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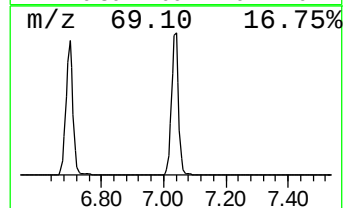
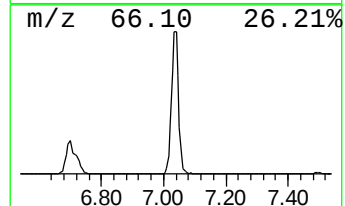
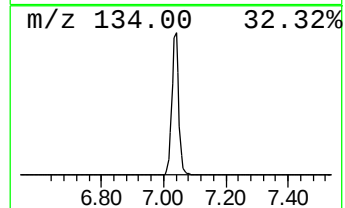
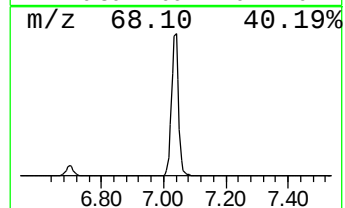
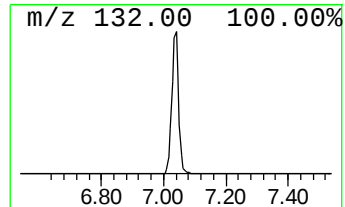
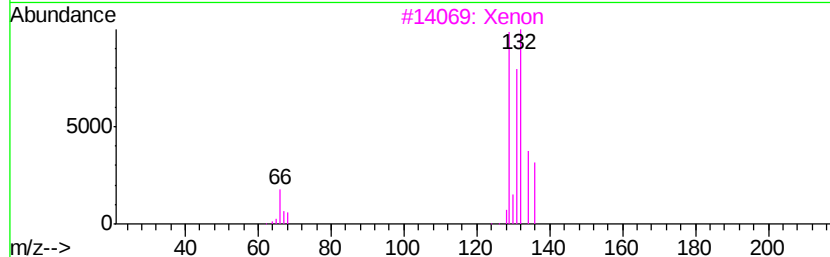
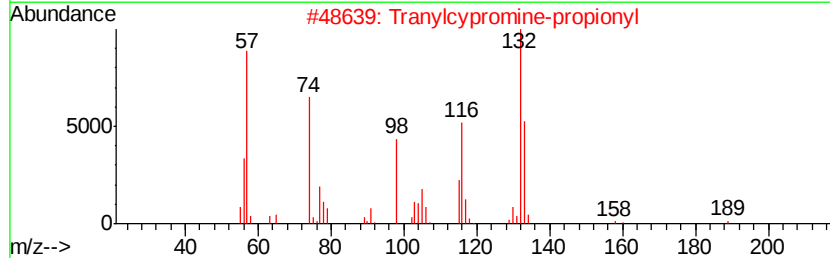
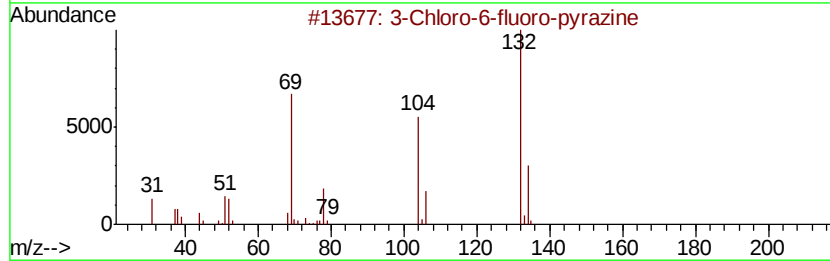
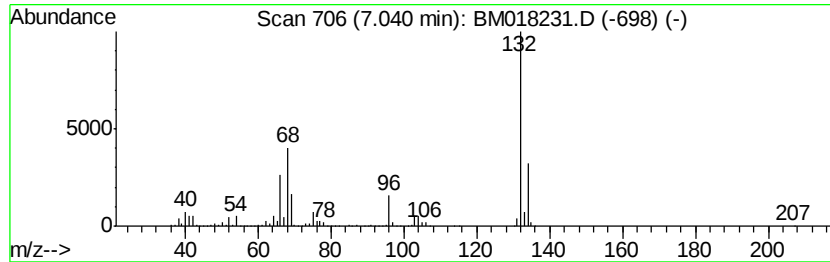
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Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	97.55 ng	3726910	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
3		Xenon	132	Xe	007440-63-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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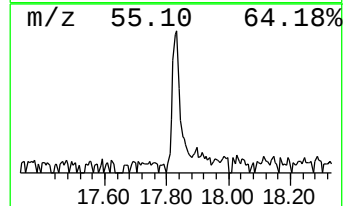
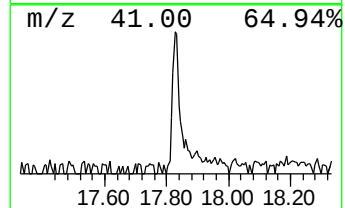
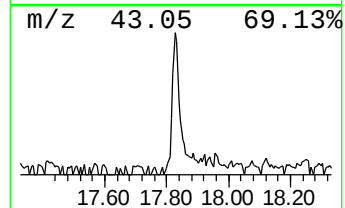
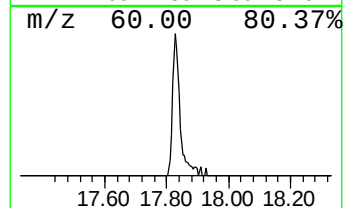
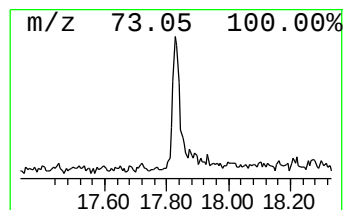
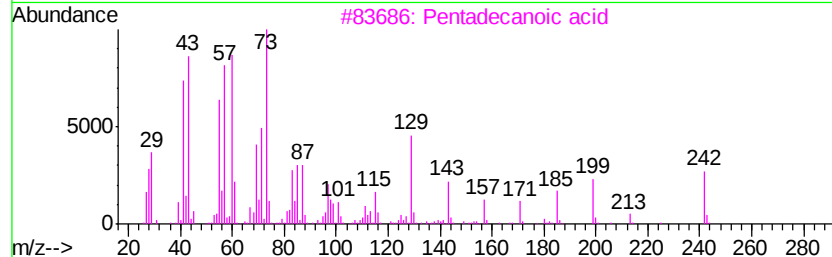
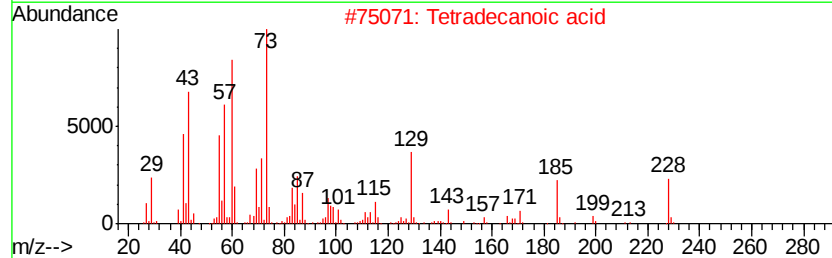
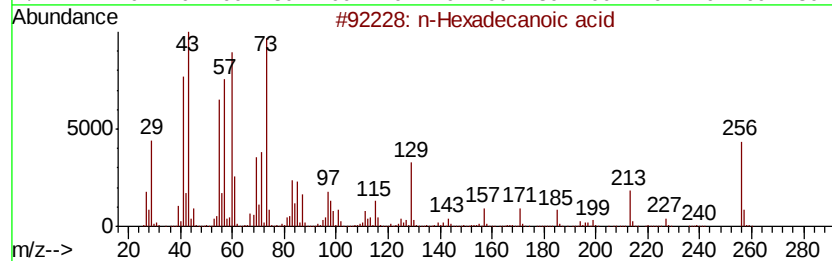
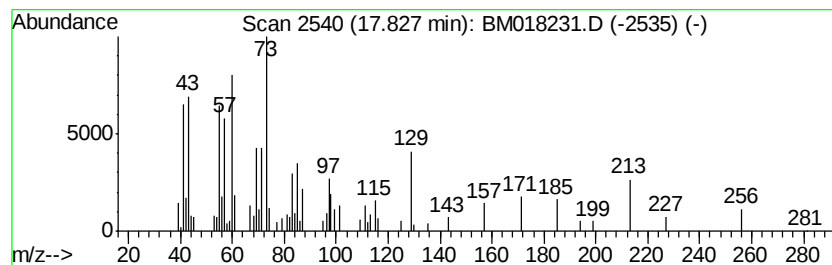
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.83	2.70 ng	165981	Phenanthrene-d10	16.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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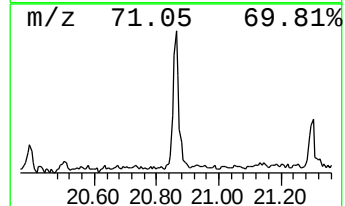
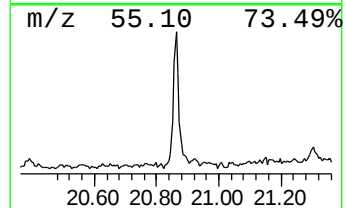
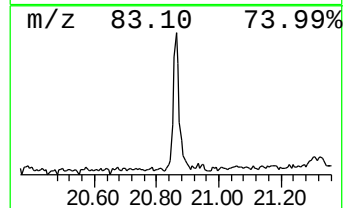
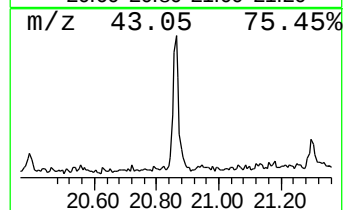
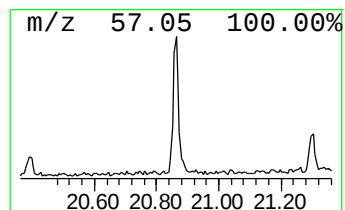
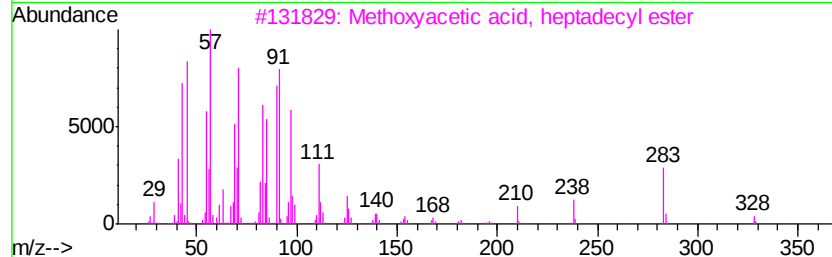
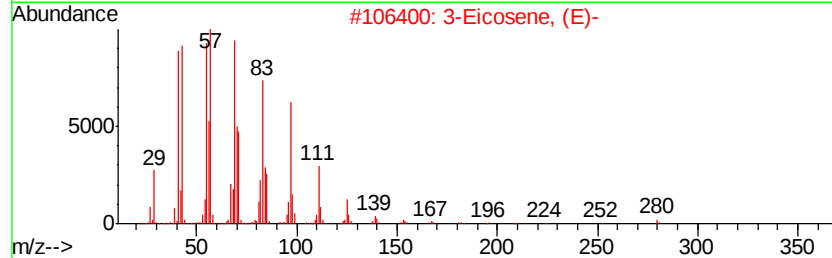
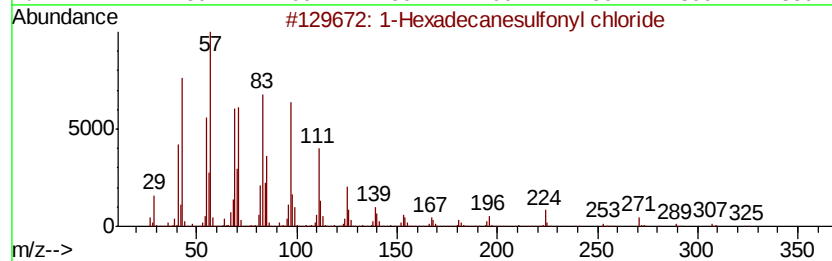
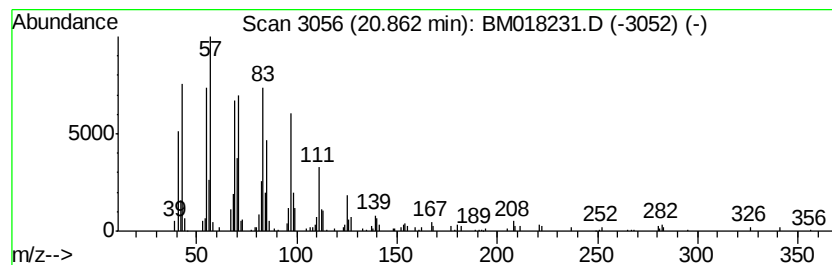
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Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.86	3.70 ng	249211	Chrysene-d12	21.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3	Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	90
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	89
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87



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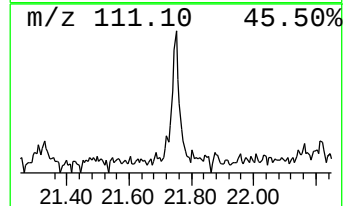
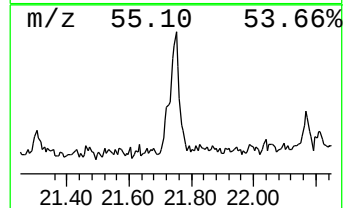
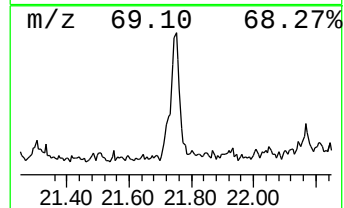
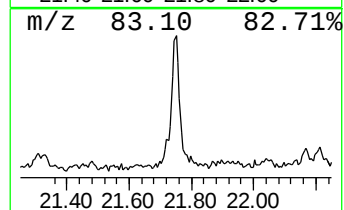
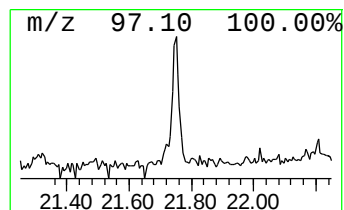
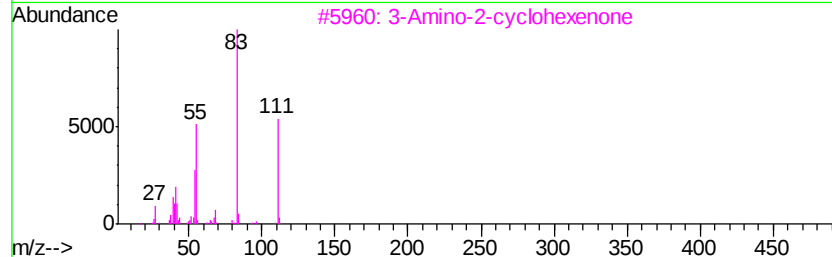
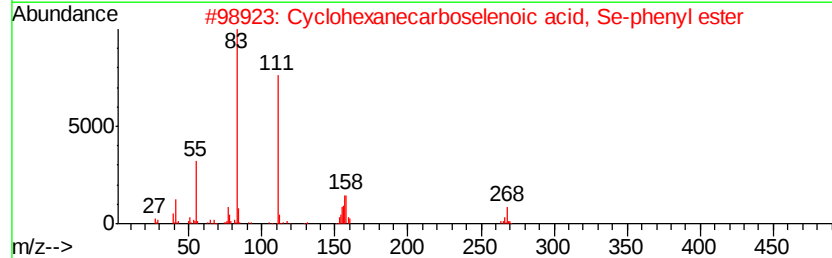
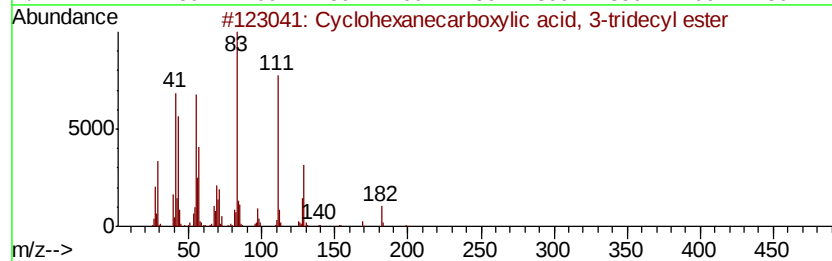
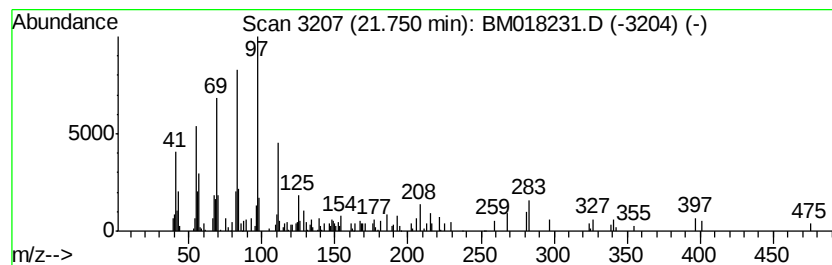
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Peak Number 6 unknown21.75 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.75	2.80 ng	188599	Chrysene-d12	21.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexanecarboxylic acid, 3-tr...	310	C20H38O2	1000280-59-4	38
2		Cyclohexanecarboxylic acid, S...	268	C13H16OSe	060718-41-4	38
3		3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	35
4		3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	30
5		3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.69	3.0	ng	116423	1	7.49	764076	20.0
unknown7.04	7.04	97.5	ng	3726910	1	7.49	764076	20.0
n-Hexadecanoic acid	17.83	2.7	ng	165981	4	16.92	1230710	20.0
1-Hexadecanesulfo...	20.86	3.7	ng	249211	5	21.14	1345630	20.0
unknown21.75	21.75	2.8	ng	188599	5	21.14	1345630	20.0