

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040717\
 Data File : BF094296.D
 Acq On : 8 Apr 2017 3:27
 Operator : SJ/MA
 Sample : I2589-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040517-PRRT-E-D-M

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-BF032217.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	3.981	352	356	362	rBV	243390	235215	5.53%	0.993%
2	4.416	426	430	440	rBV	1141585	1183375	27.85%	4.997%
3	5.492	609	613	623	rVB	748042	764742	17.99%	3.229%
4	5.610	629	633	637	rBV	2421569	2259335	53.16%	9.540%
5	5.851	670	674	678	rBV	928864	820454	19.31%	3.464%
6	6.034	700	705	708	rBV	3217869	3167684	74.54%	13.375%
7	6.504	778	785	788	rBV	2165516	2563058	60.31%	10.822%
8	7.357	925	930	933	rBV	1066073	1021101	24.03%	4.311%
9	8.681	1149	1155	1159	rBV	3940112	4249767	100.00%	17.944%
10	9.175	1235	1239	1243	rBV	116112	99487	2.34%	0.420%
11	9.492	1290	1293	1298	rVB2	890873	922918	21.72%	3.897%
12	10.086	1389	1394	1399	rVB	54820	49446	1.16%	0.209%
13	10.475	1455	1460	1464	rBV	1181896	1209287	28.46%	5.106%
14	10.669	1489	1493	1502	rBV	58670	78513	1.85%	0.332%
15	11.316	1599	1603	1608	rBV	699336	720344	16.95%	3.041%
16	13.304	1935	1941	1944	rBV	2455115	2776480	65.33%	11.723%
17	14.574	2152	2157	2161	rBV	721890	761752	17.92%	3.216%
18	16.204	2429	2434	2438	rBV	550753	629888	14.82%	2.660%
19	16.315	2450	2453	2457	rBV2	41684	50805	1.20%	0.215%
20	16.715	2518	2521	2526	rBV3	38994	53033	1.25%	0.224%
21	17.698	2684	2688	2694	rVB4	36535	67233	1.58%	0.284%

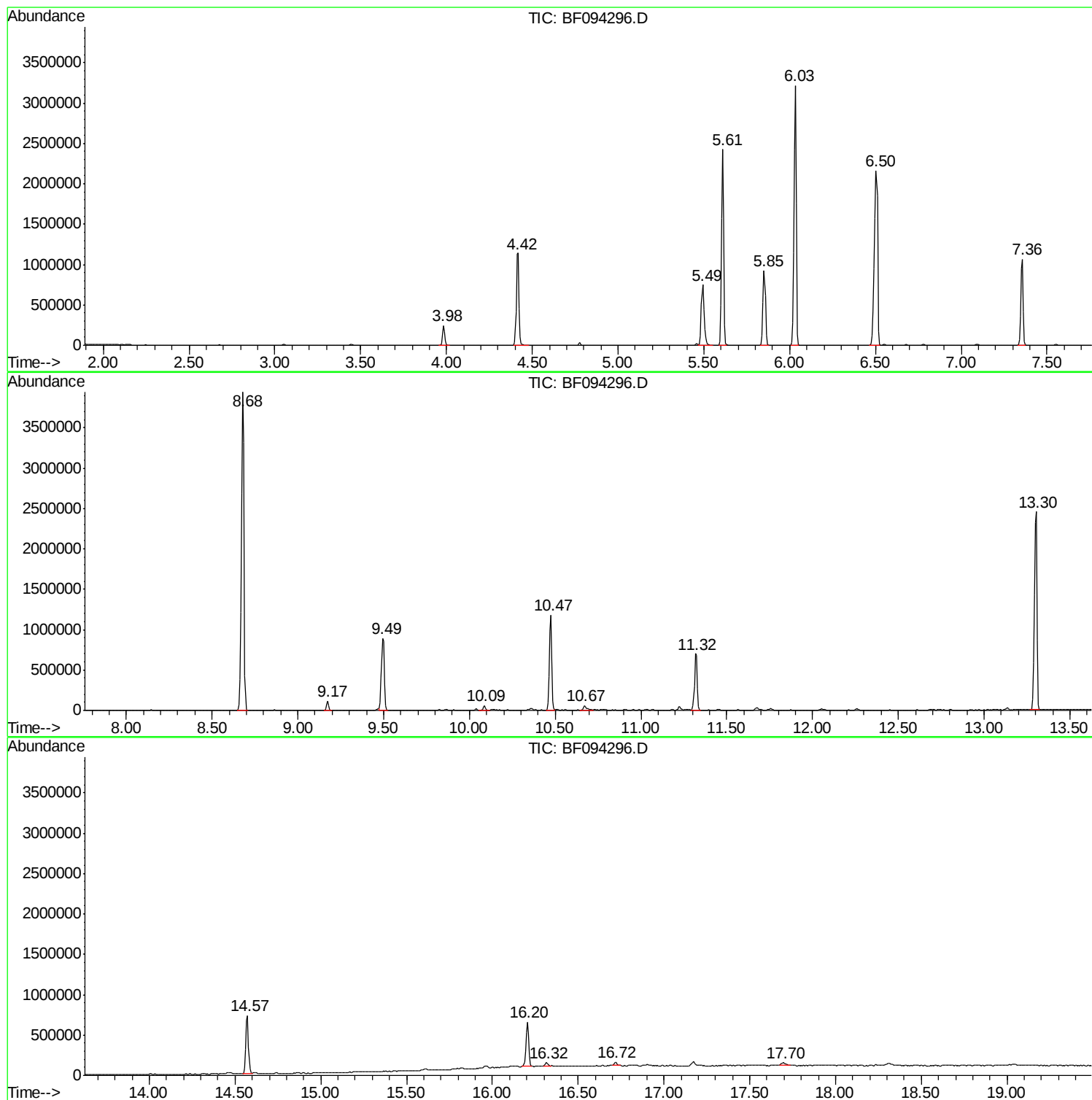
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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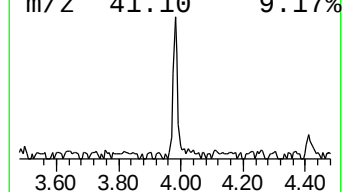
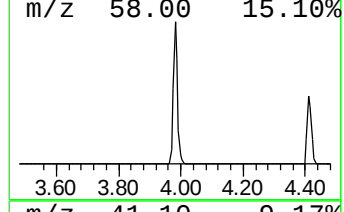
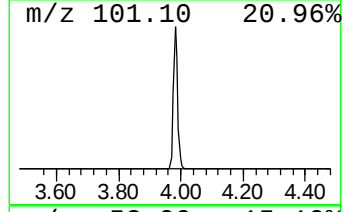
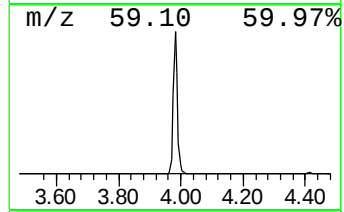
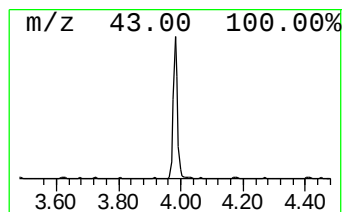
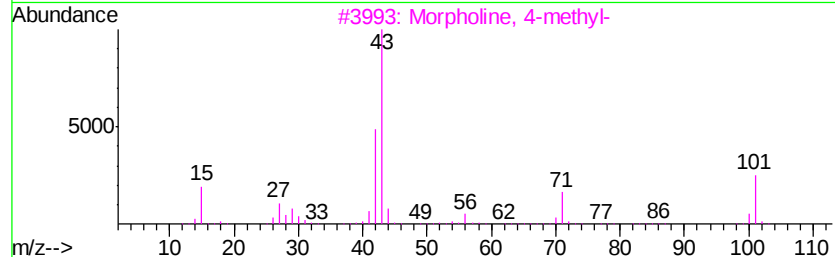
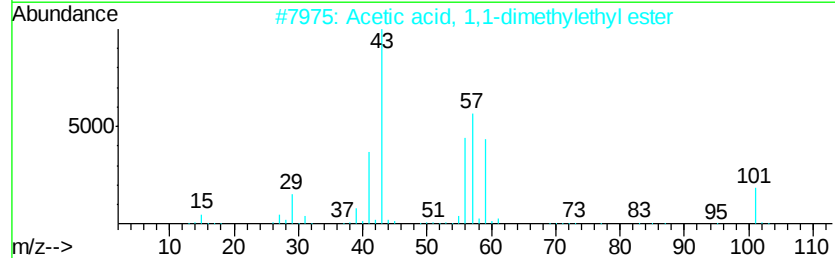
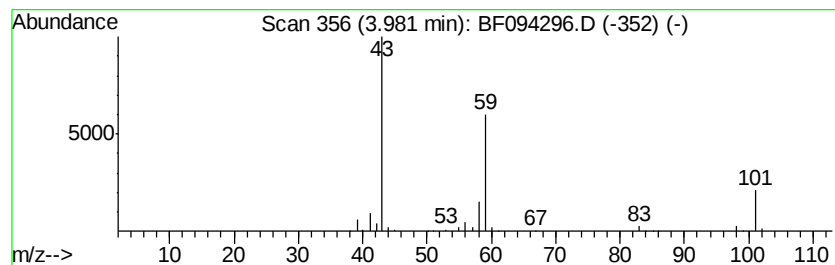
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	5.73 ng	235215	1,4-Dichlorobenzene-d4	5.85

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	39		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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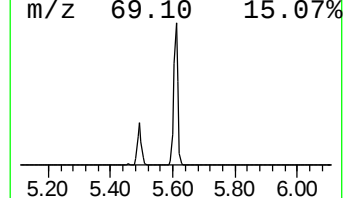
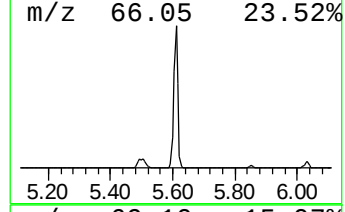
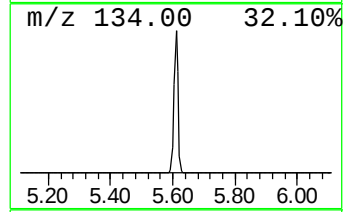
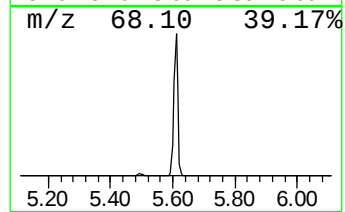
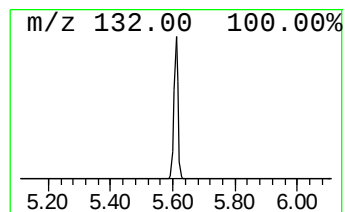
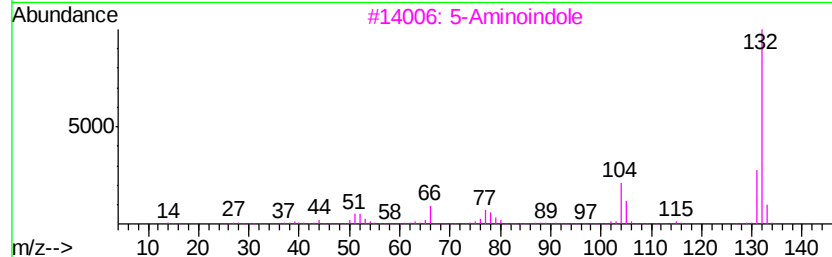
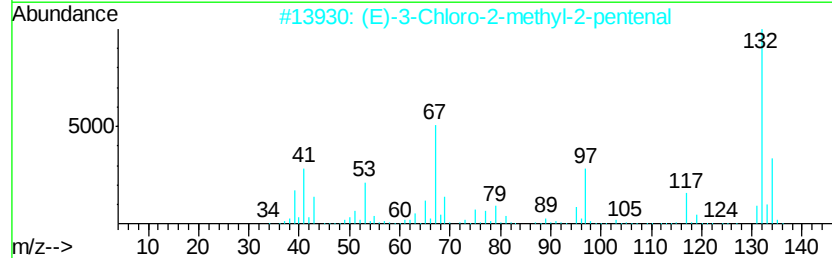
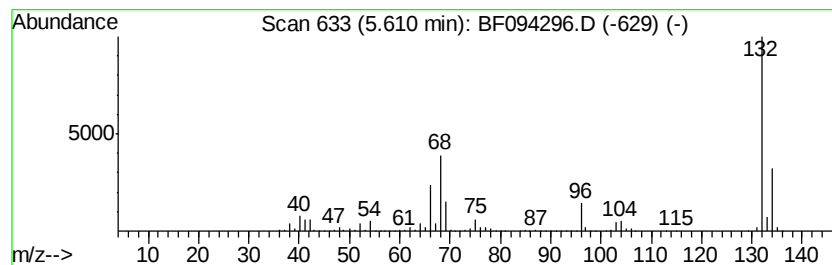
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Peak Number 2 unknown5.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	55.08 ng	2259340	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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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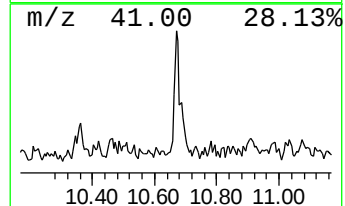
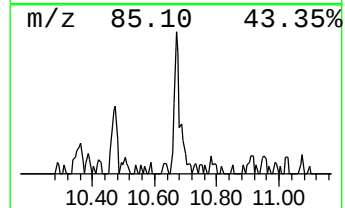
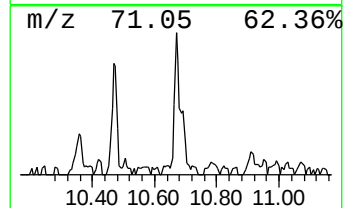
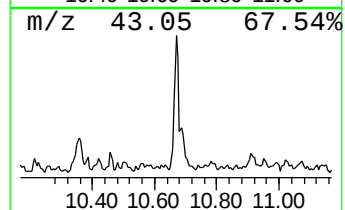
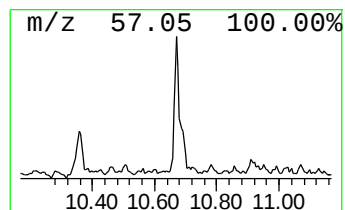
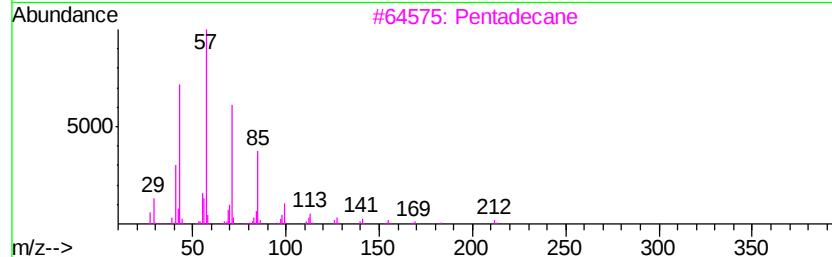
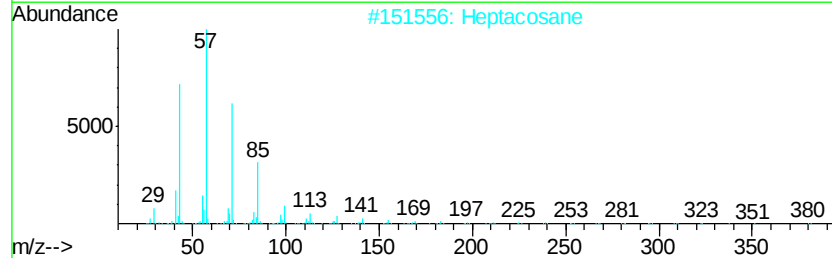
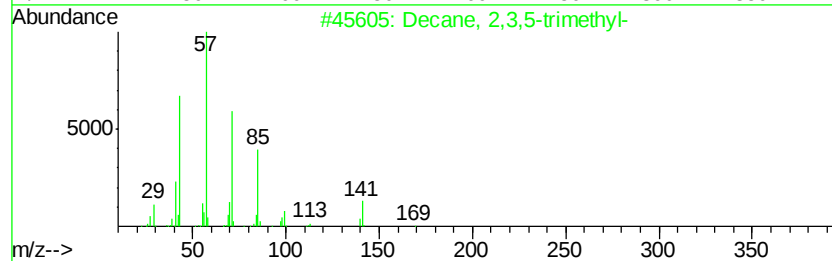
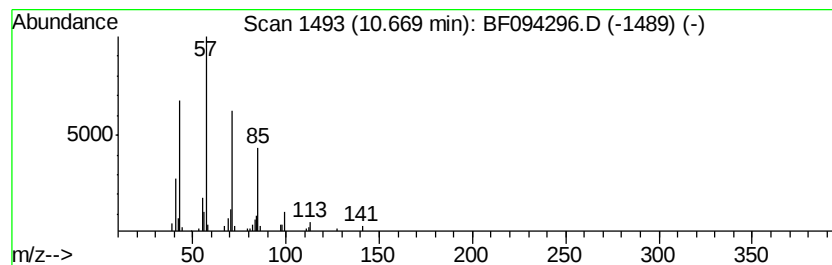
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Peak Number 4 Decane, 2,3,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.18 ng	78513	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2		Heptacosane	380	C27H56	000593-49-7	86
3		Pentadecane	212	C15H32	000629-62-9	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Hexadecane	226	C16H34	000544-76-3	78



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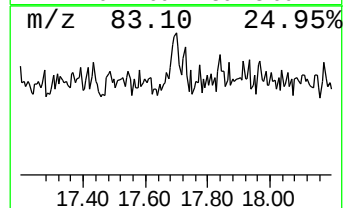
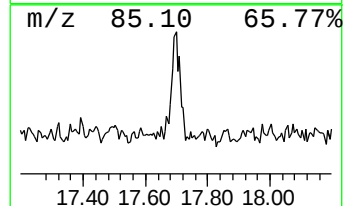
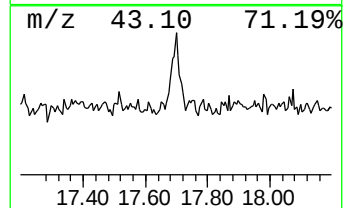
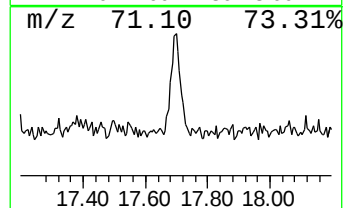
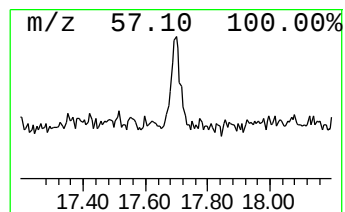
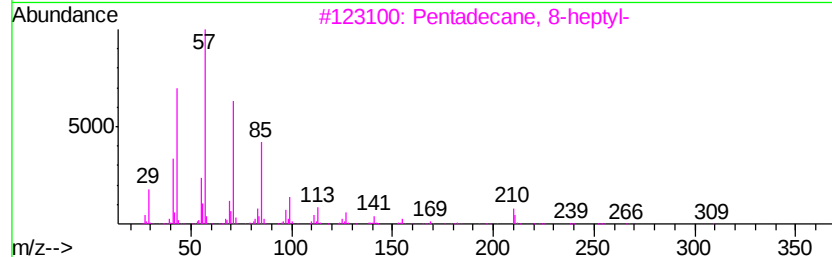
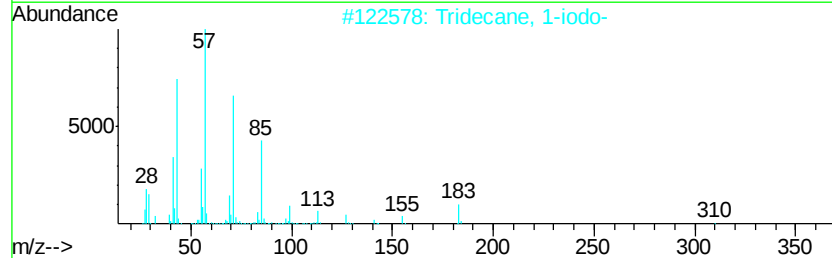
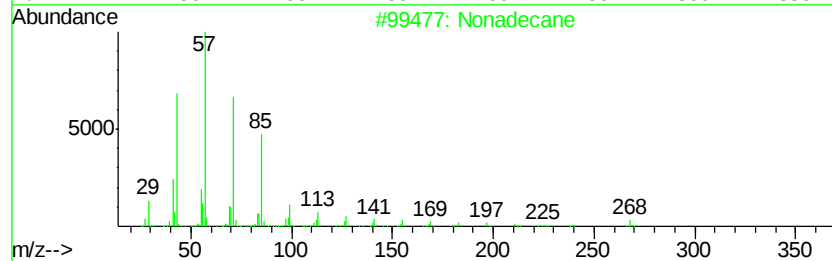
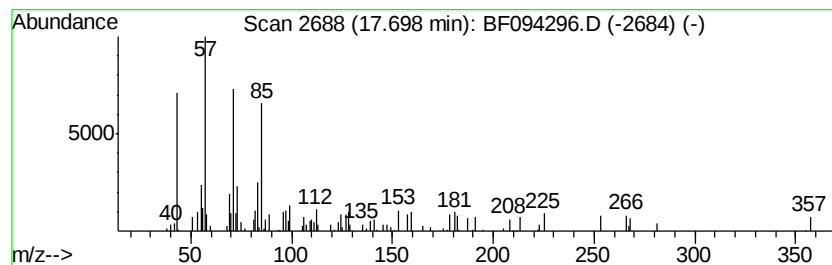
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Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	2.13 ng	67233	Perylene-d12	16.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	64
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	50
3	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	50
4	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	50
5	Decane, 3-bromo-		220	C10H21Br	030571-71-2	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.98	5.7	ng	235215	1	5.85	820454	20.0
unknown5.61	5.61	55.1	ng	2259340	1	5.85	820454	20.0
Decane, 2,3,5-tri...	10.67	2.2	ng	78513	4	11.32	720344	20.0
Nonadecane	17.70	2.1	ng	67233	6	16.20	629888	20.0