

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
 Data File : BF103289.D
 Acq On : 28 Feb 2018 3:47
 Operator : SJ/JU
 Sample : J1683-01
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RFK-RMAB-MW06-GW

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-BF022218.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	2.140	3	9	17	rBV	895446	1202796	30.32%	4.141%
2	3.593	246	256	260	rBV2	31917	58836	1.48%	0.203%
3	3.728	268	279	285	rVB	82503	147881	3.73%	0.509%
4	5.093	508	511	519	rBV	110888	126948	3.20%	0.437%
5	5.493	576	579	600	rBV	2106470	2286175	57.63%	7.870%
6	6.251	706	708	713	rVB	56245	47998	1.21%	0.165%
7	6.504	747	751	764	rBV	1213907	1343472	33.87%	4.625%
8	6.645	770	775	778	rBV	3515168	3320214	83.70%	11.430%
9	6.816	798	804	810	rBV	40104	45505	1.15%	0.157%
10	6.869	810	813	817	rBV	957034	866835	21.85%	2.984%
11	6.910	817	820	830	rVB2	63170	80907	2.04%	0.279%
12	7.034	836	841	844	rBV	3176618	3252986	82.00%	11.199%
13	7.439	902	910	913	rBV	2679844	2835255	71.47%	9.761%
14	8.157	1028	1032	1042	rBV	1133489	1102792	27.80%	3.797%
15	9.233	1210	1215	1218	rBV	3950079	3966833	100.00%	13.656%
16	9.622	1277	1281	1286	rBV	95145	88827	2.24%	0.306%
17	9.828	1312	1316	1320	rBV	82036	69749	1.76%	0.240%
18	9.910	1327	1330	1338	rVB	1103191	1027240	25.90%	3.536%
19	10.322	1397	1400	1404	rVB2	226809	230842	5.82%	0.795%
20	10.545	1433	1438	1441	rBV	34288	45285	1.14%	0.156%
21	10.704	1461	1465	1475	rBV	1717271	1851693	46.68%	6.375%
22	10.804	1479	1482	1486	rVV	91361	94456	2.38%	0.325%
23	11.404	1580	1584	1592	rBV	890937	838552	21.14%	2.887%
24	11.951	1675	1677	1685	rVB	48658	46859	1.18%	0.161%
25	12.851	1825	1830	1837	rBV3	28315	42378	1.07%	0.146%
26	12.992	1849	1854	1857	rBV	2730896	2734679	68.94%	9.415%
27	13.868	2000	2003	2013	rBV	44265	55266	1.39%	0.190%
28	14.051	2030	2034	2044	rBV	700474	681731	17.19%	2.347%
29	15.551	2284	2289	2296	rBV	378315	554502	13.98%	1.909%

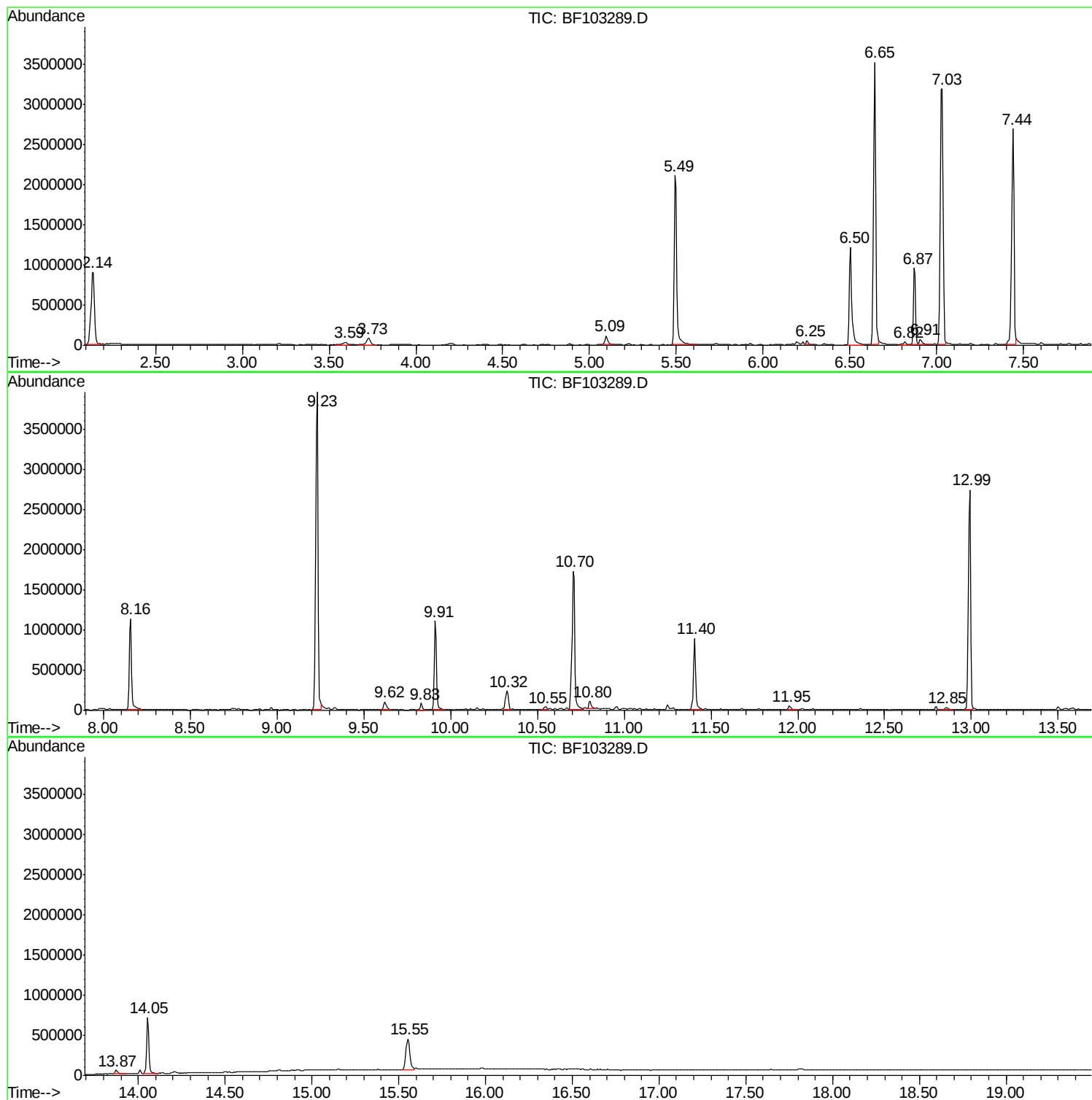
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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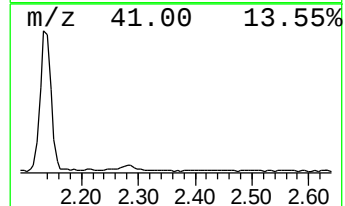
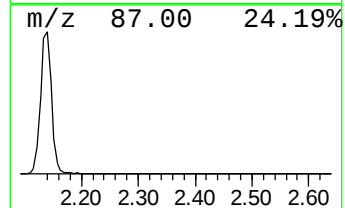
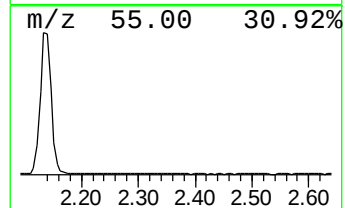
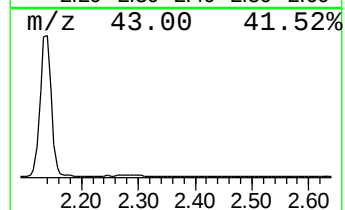
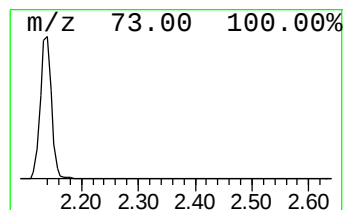
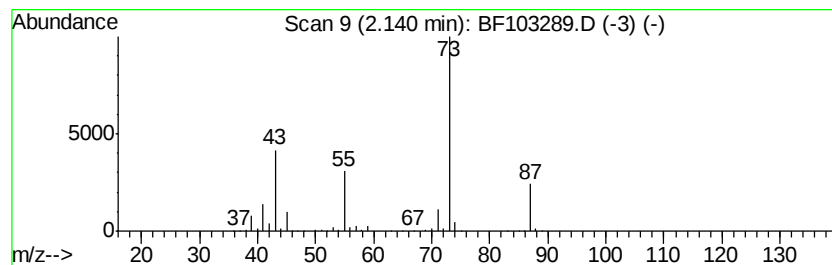
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	27.75 ng	1202800	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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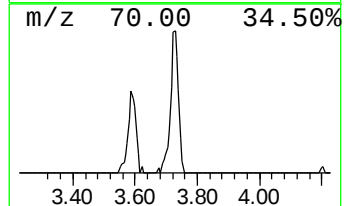
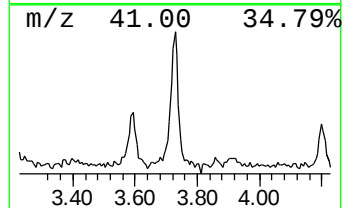
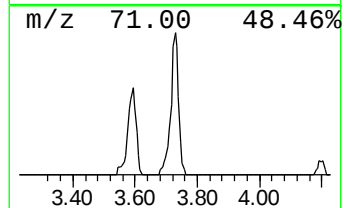
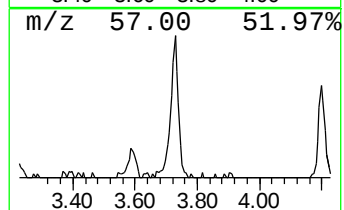
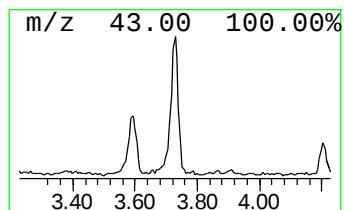
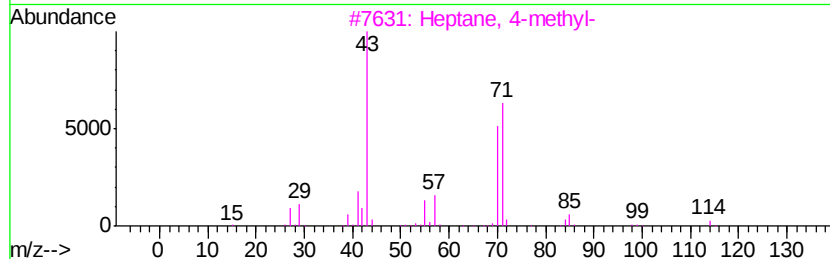
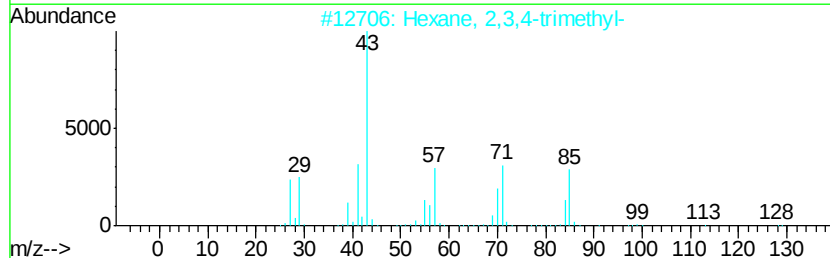
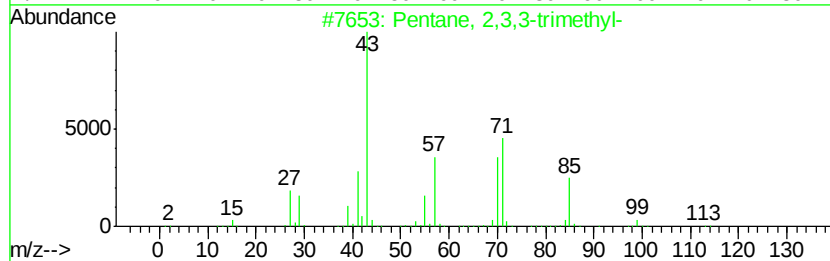
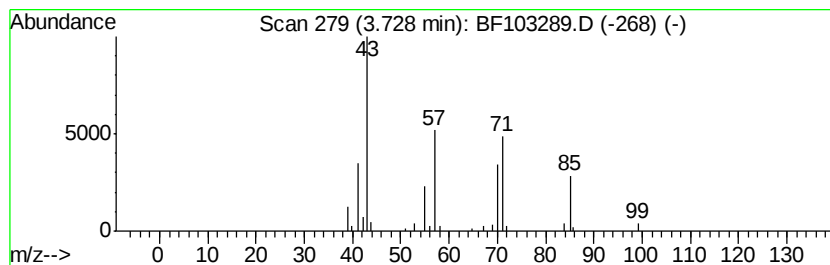
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	3.41 ng	147881	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	56
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53



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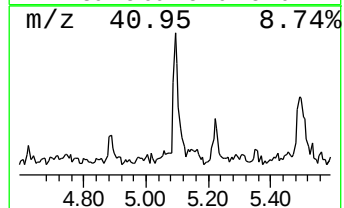
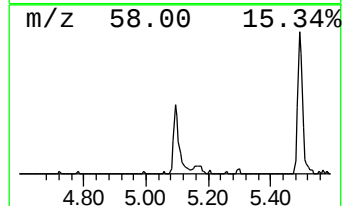
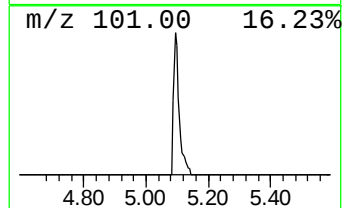
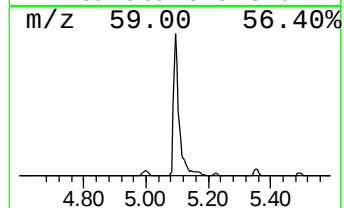
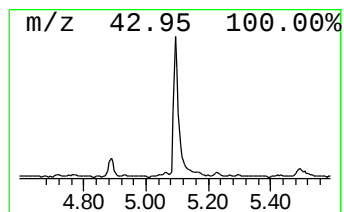
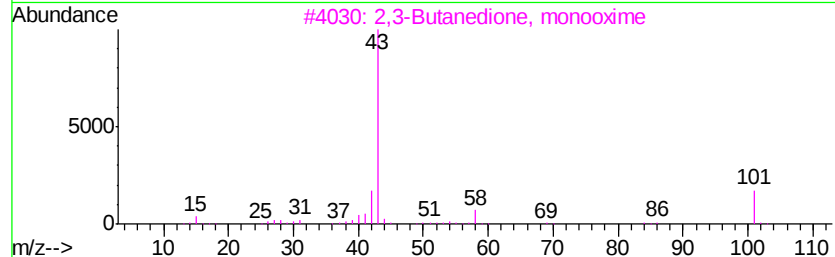
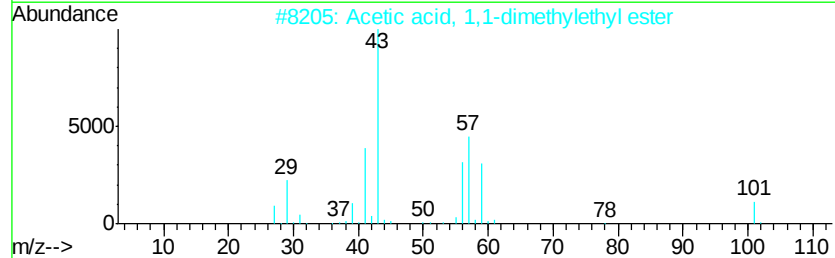
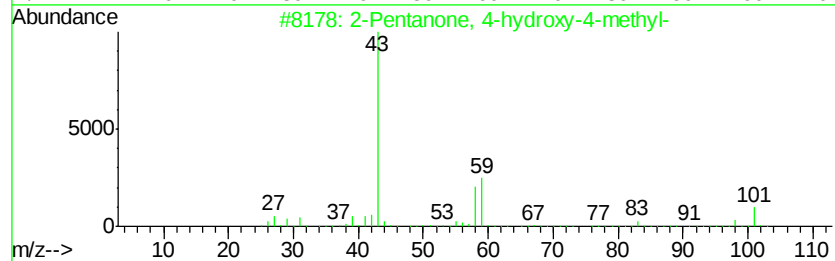
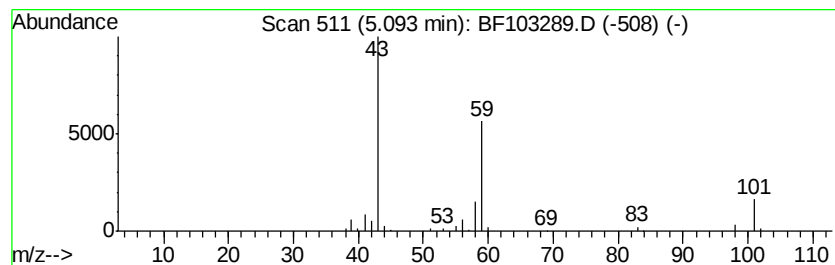
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.93 ng	126948	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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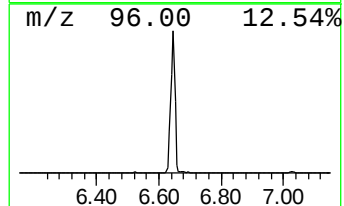
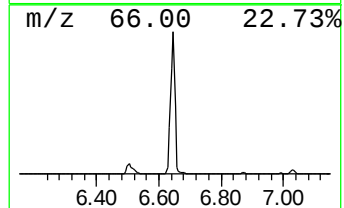
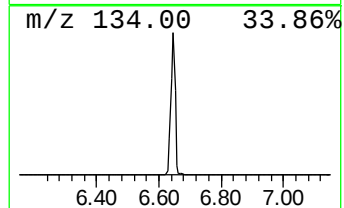
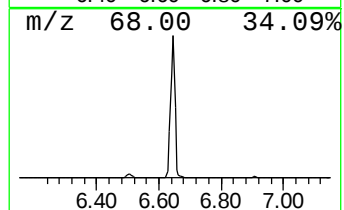
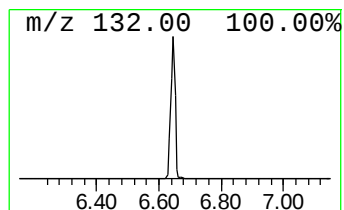
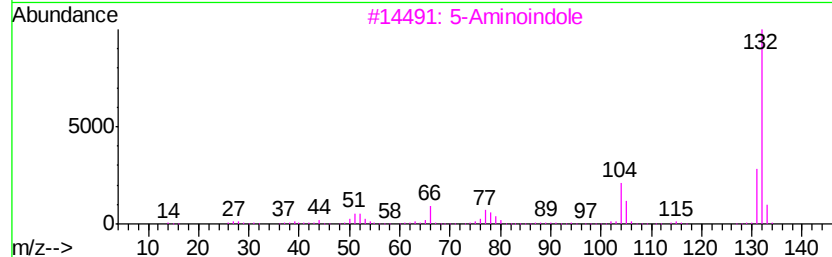
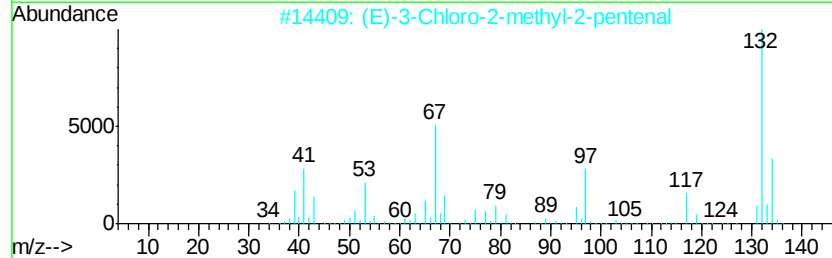
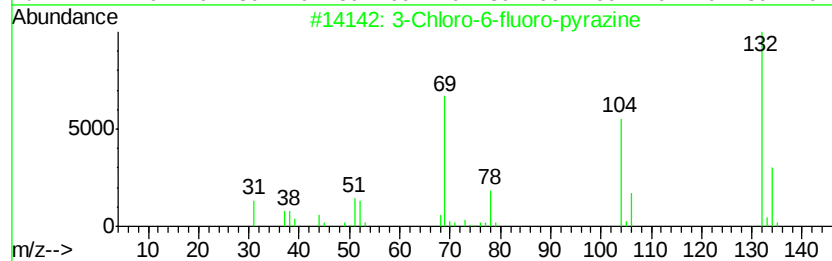
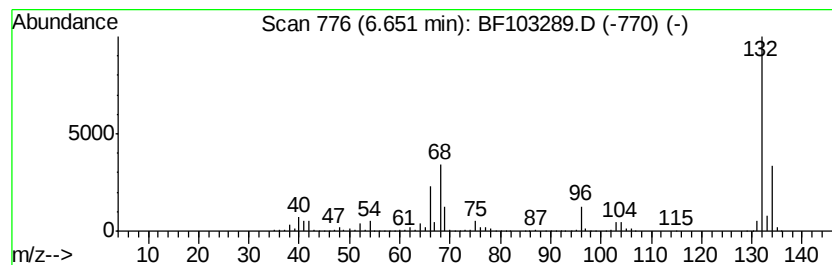
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Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	76.61 ng	3320210	1,4-Dichlorobenzene-d4	6.87

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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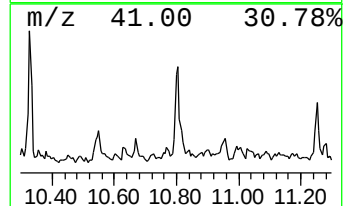
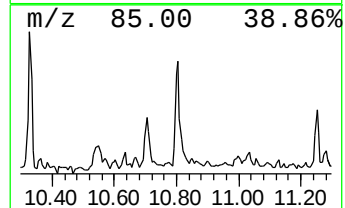
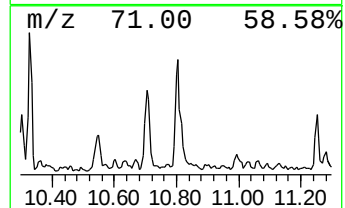
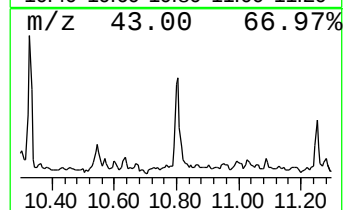
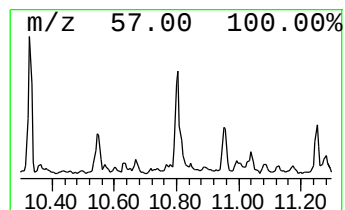
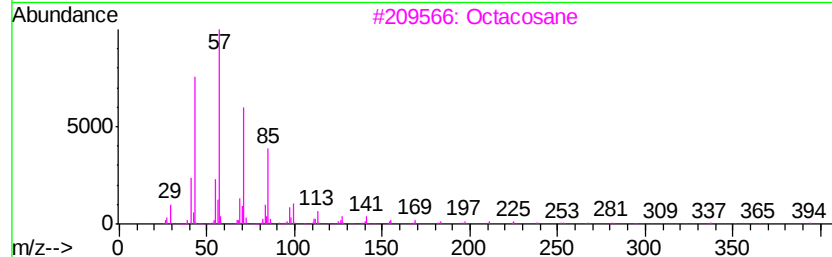
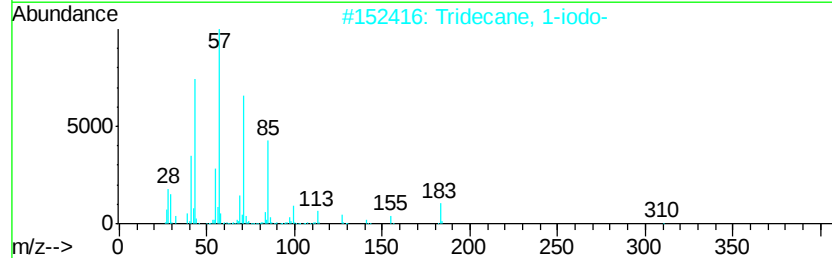
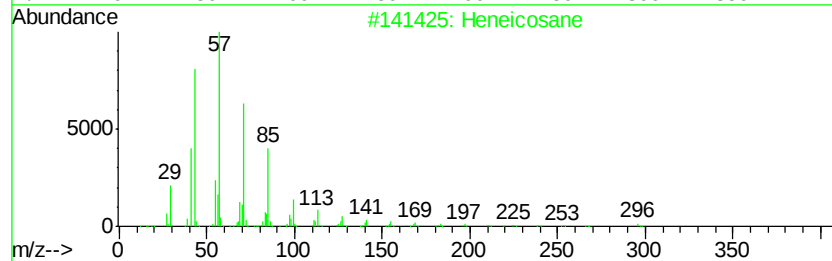
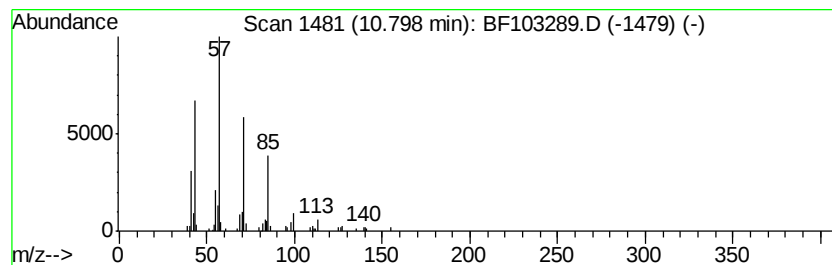
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Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.80	2.25 ng	94456	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetradecane	198	C14H30	000629-59-4	90
5	Hexadecane	226	C16H34	000544-76-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	27.8	ng	1202800	1	6.87	866835	20.0
Pentane, 2,3,3-tr...	3.73	3.4	ng	147881	1	6.87	866835	20.0
2-Pentanone, 4-hy...	5.09	2.9	ng	126948	1	6.87	866835	20.0
unknown6.65	6.65	76.6	ng	3320210	1	6.87	866835	20.0
Heneicosane	10.80	2.3	ng	94456	4	11.40	838552	20.0