

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010820\
 Data File : BG043974.D
 Acq On : 8 Jan 2020 19:22
 Operator : JU
 Sample : PB125951BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB125951BL

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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	3.138	3	8	47	rVB	2107605	4839575	61.95%	10.823%
2	5.065	330	336	349	rVB	237312	412007	5.27%	0.921%
3	5.535	409	416	436	rBV	1233107	2174575	27.84%	4.863%
4	7.122	675	686	702	rBV	850859	1527538	19.55%	3.416%
5	7.492	740	749	763	rBV	1967701	3700912	47.37%	8.277%
6	7.956	821	828	836	rBV	420820	744209	9.53%	1.664%
7	8.279	872	883	898	rBV	1561926	2846991	36.44%	6.367%
8	9.108	1013	1024	1043	rBV	1219374	2337761	29.93%	5.228%
9	10.753	1297	1304	1316	rBV	541152	1019616	13.05%	2.280%
10	13.214	1715	1723	1734	rBV	3138358	5211729	66.71%	11.655%
11	14.589	1950	1957	1968	rBV	891061	1470094	18.82%	3.288%
12	16.076	2202	2210	2227	rBV	2703452	4375462	56.01%	9.785%
13	17.327	2416	2423	2435	rBV	1128918	1759008	22.52%	3.934%
14	19.948	2862	2869	2881	rBV	5440367	7812007	100.00%	17.471%
15	21.581	3139	3147	3158	rBV2	1012233	1762544	22.56%	3.942%
16	21.793	3179	3183	3190	rBV	50268	79517	1.02%	0.178%
17	22.392	3280	3285	3292	rVB2	83273	142075	1.82%	0.318%
18	23.068	3395	3400	3405	rVB	94318	163099	2.09%	0.365%
19	23.855	3528	3534	3543	rVB2	91417	198682	2.54%	0.444%
20	24.701	3667	3678	3687	rBV2	623445	1773180	22.70%	3.966%
21	24.777	3687	3691	3700	rVB3	88156	212181	2.72%	0.475%
22	25.876	3873	3878	3888	rVB4	55770	152222	1.95%	0.340%

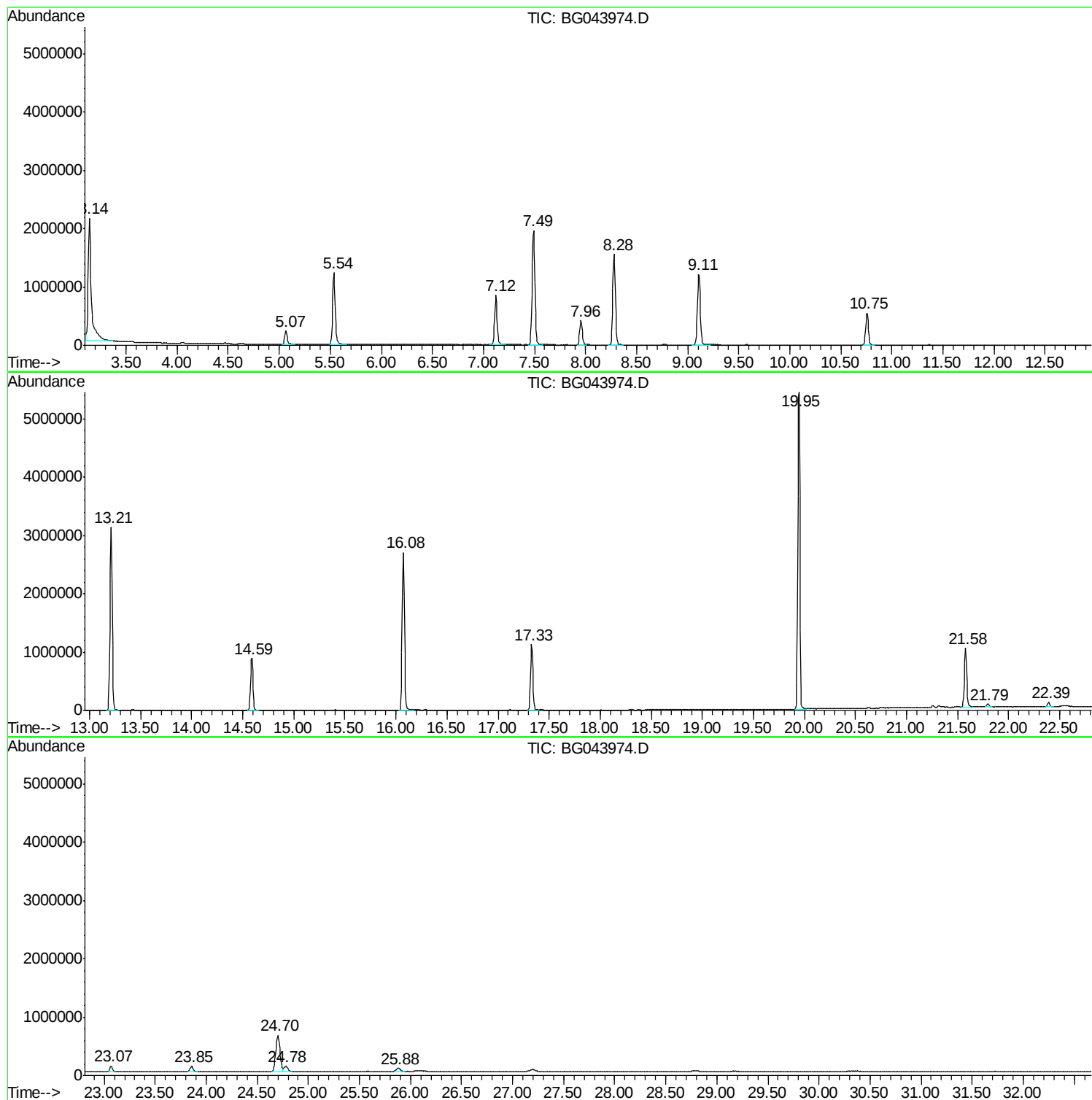
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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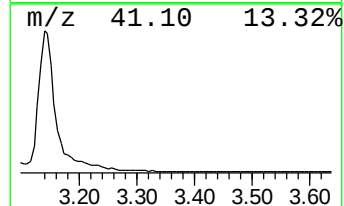
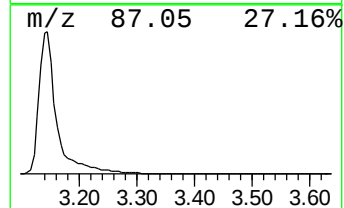
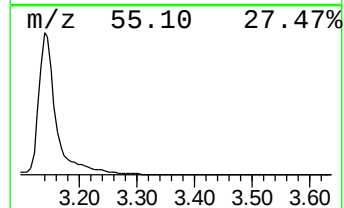
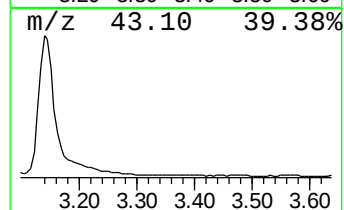
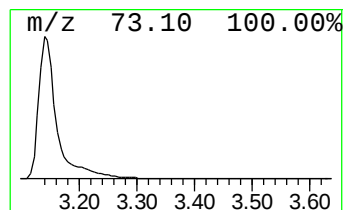
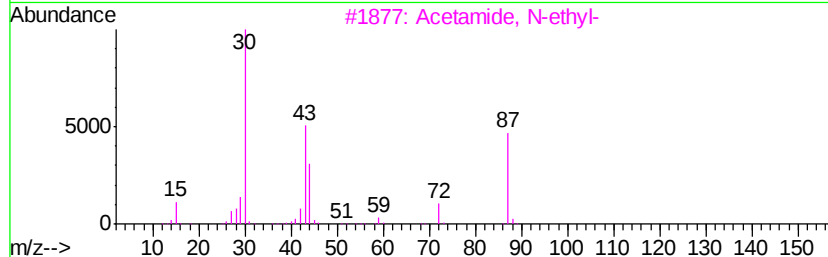
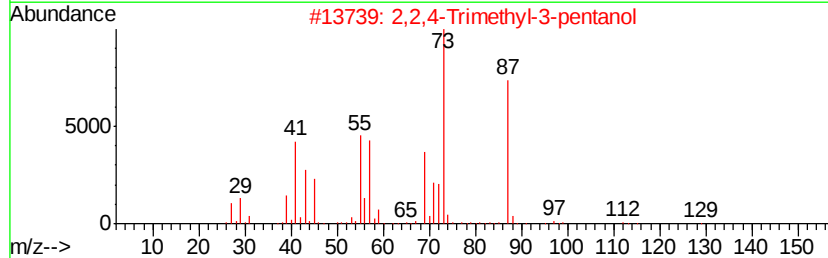
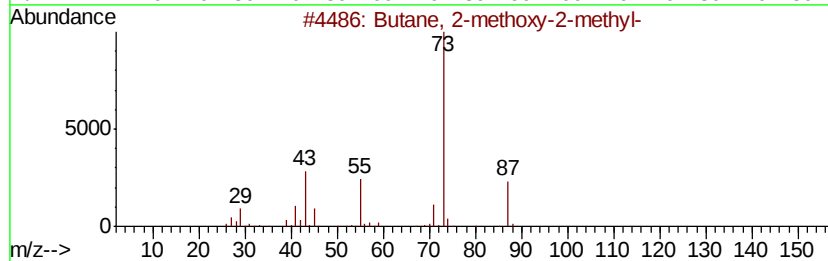
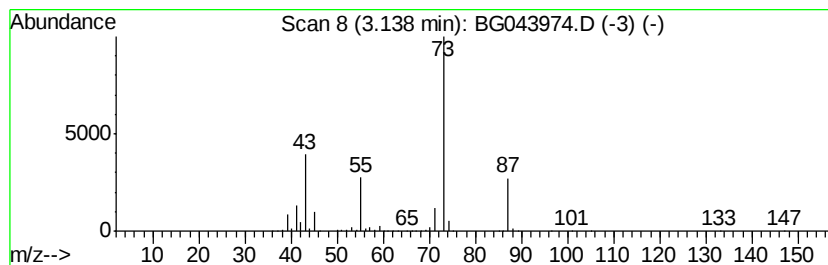
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	130.06 ng	4839580	1,4-Dichlorobenzene-d4	7.96

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	38
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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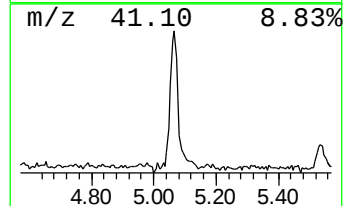
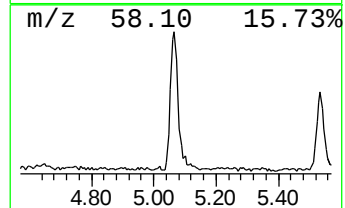
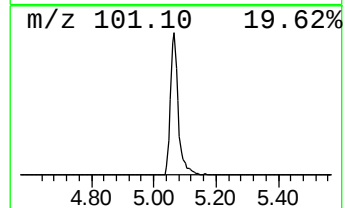
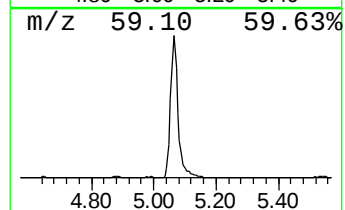
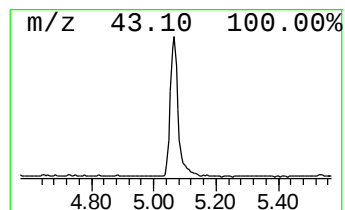
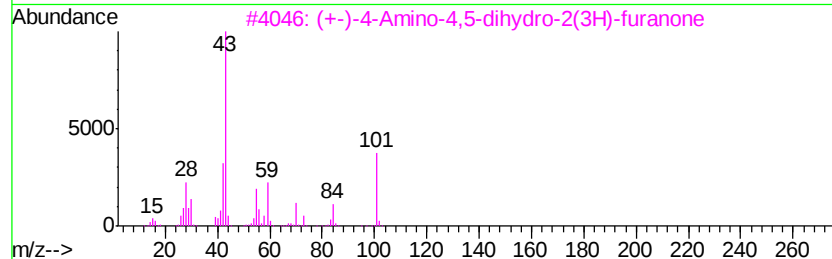
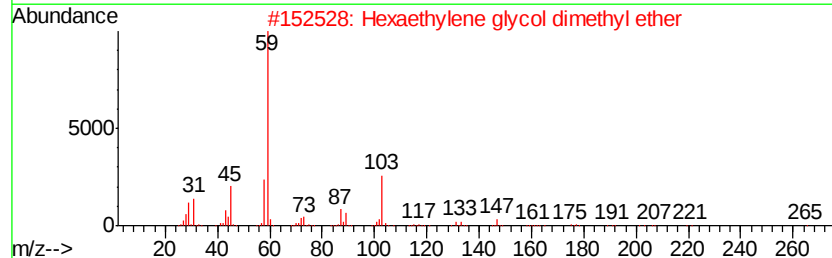
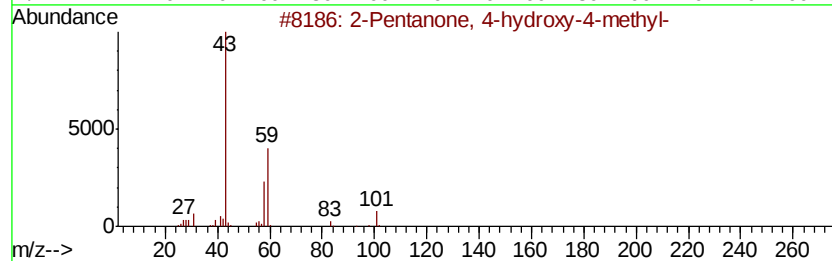
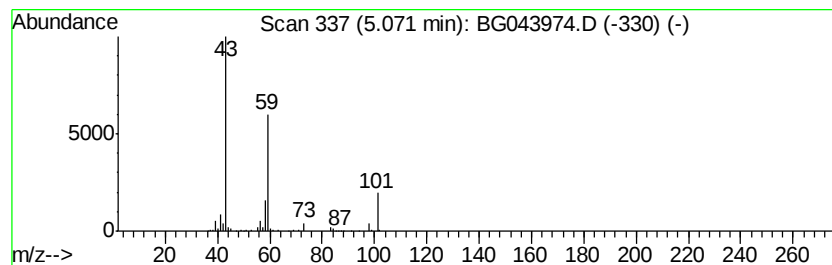
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	11.07 ng	412007	1,4-Dichlorobenzene-d4	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	32
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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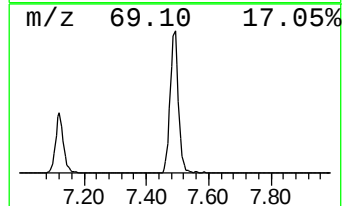
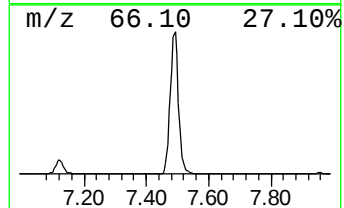
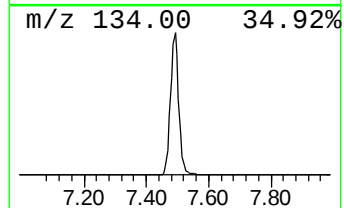
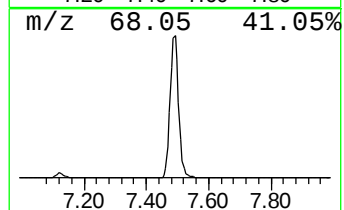
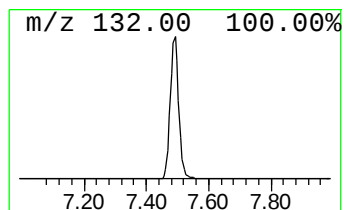
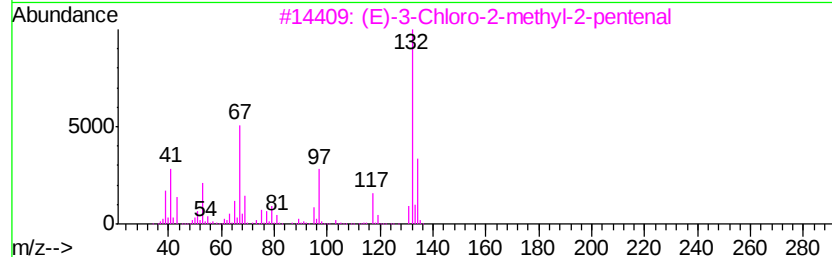
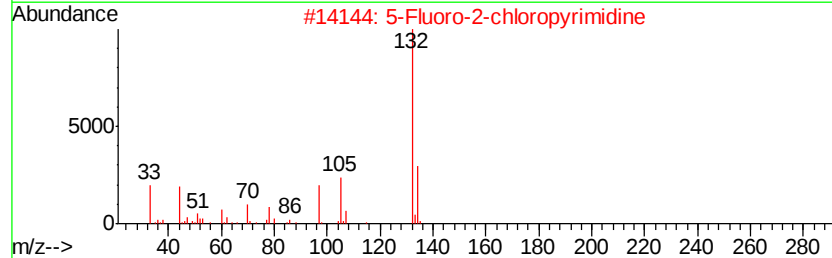
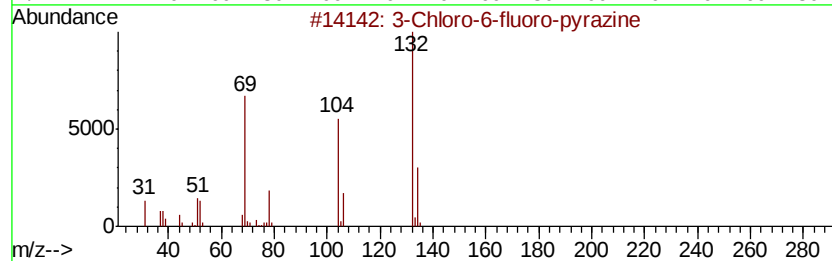
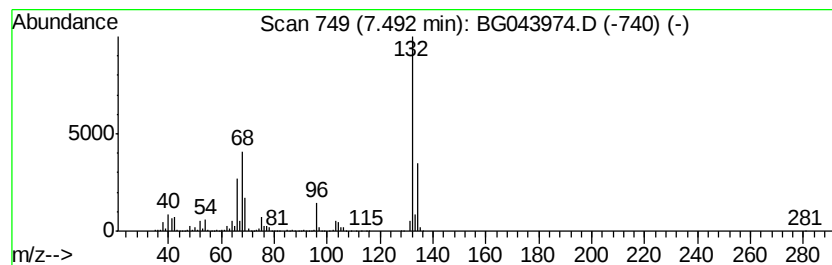
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	99.46 ng	3700910	1,4-Dichlorobenzene-d4	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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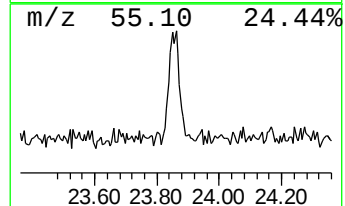
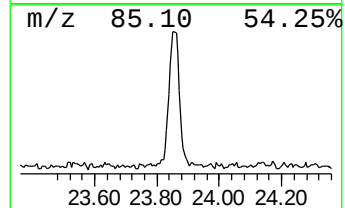
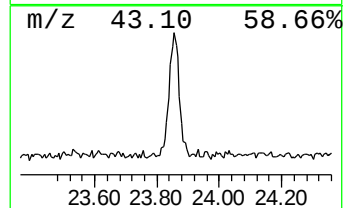
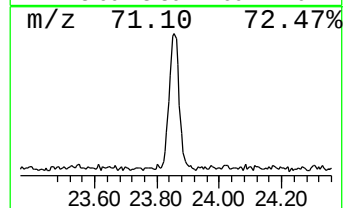
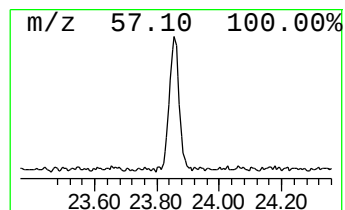
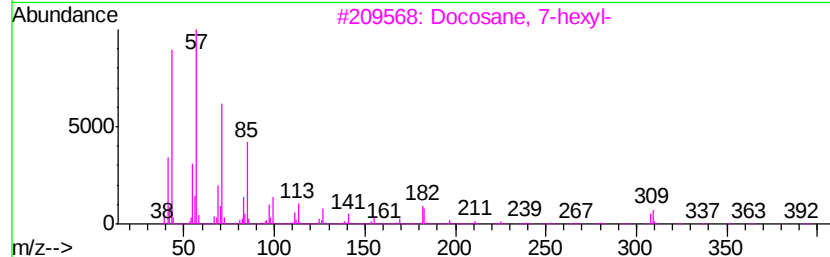
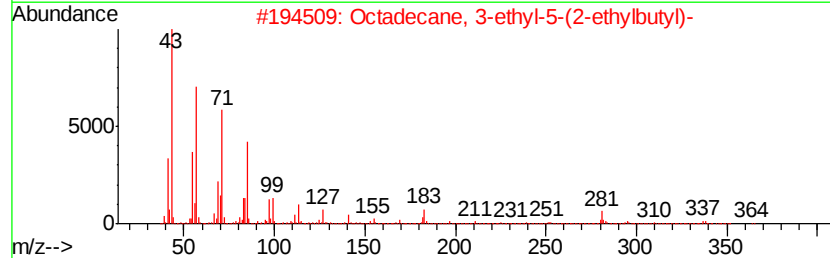
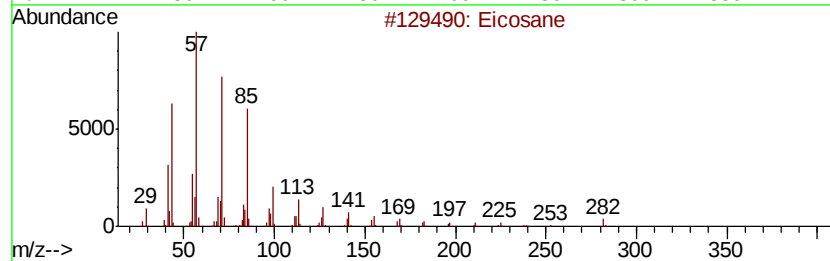
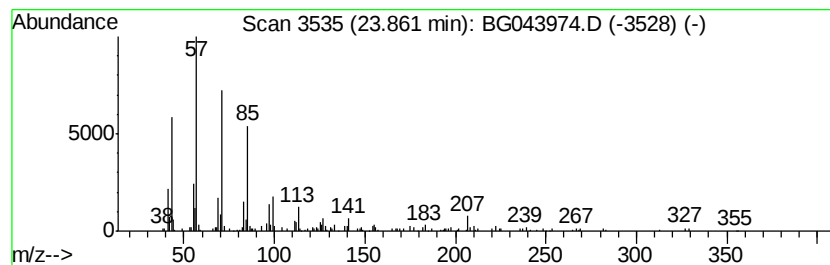
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.86	2.24 ng	198682	Perylene-d12	24.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Octadecane, 3-ethyl-5-(2-ethylbu...		366	C26H54	055282-12-7	90
3	Docosane, 7-hexyl-		394	C28H58	055373-86-9	87
4	Hexatriacontane		507	C36H74	000630-06-8	87
5	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	87



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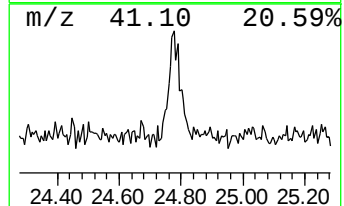
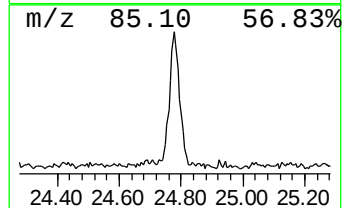
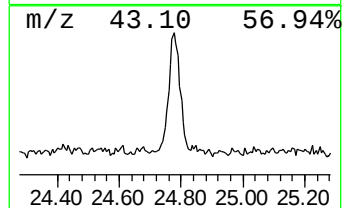
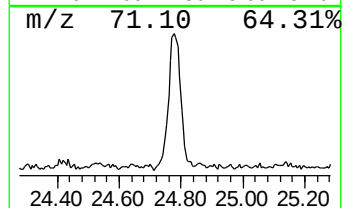
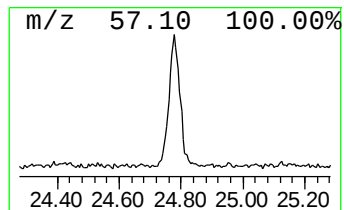
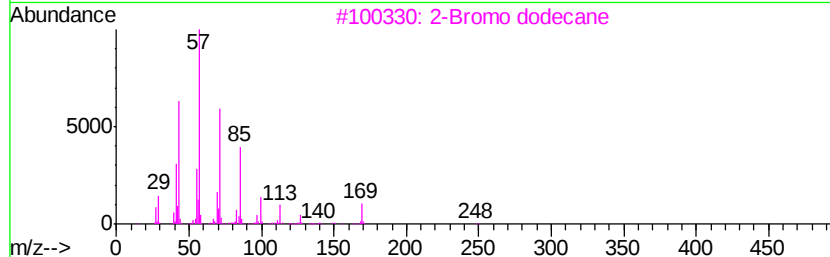
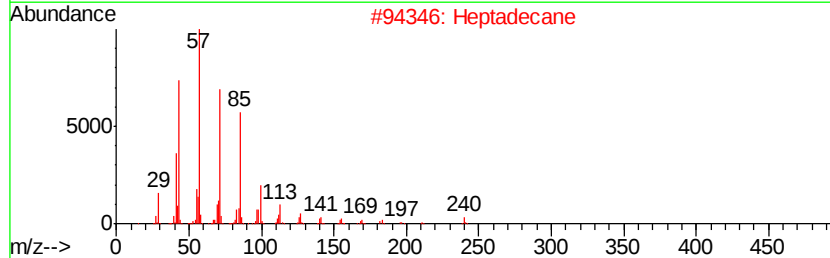
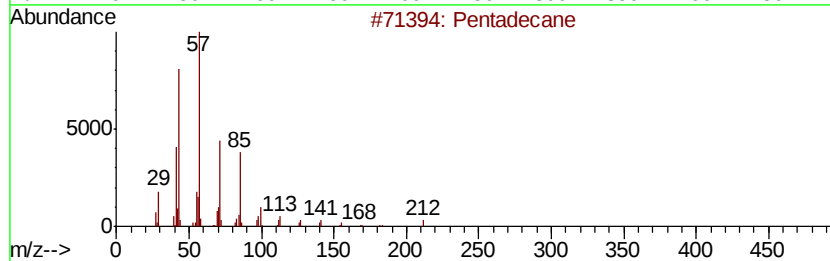
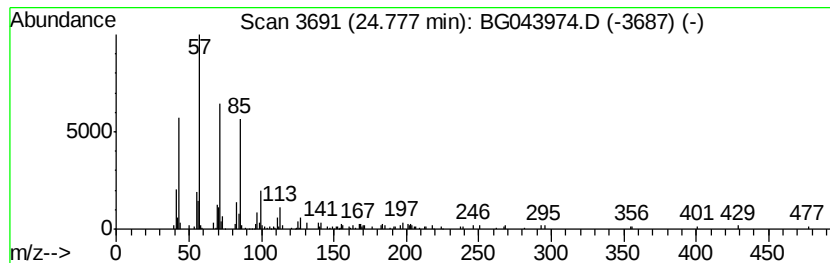
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Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.78	2.39 ng	212181	Perylene-d12	24.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	90
2		Heptadecane	240	C17H36	000629-78-7	86
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4		Pentacosane	352	C25H52	000629-99-2	86
5		Nonadecane	268	C19H40	000629-92-5	80



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.14	130.1	ng	4839580	1	7.96	744209	20.0
2-Pentanone, 4-hy...	5.07	11.1	ng	412007	1	7.96	744209	20.0
unknown7.49	7.49	99.5	ng	3700910	1	7.96	744209	20.0
Eicosane	23.86	2.2	ng	198682	6	24.70	1773180	20.0
Pentadecane	24.78	2.4	ng	212181	6	24.70	1773180	20.0