

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080918\
 Data File : BF108042.D
 Acq On : 9 Aug 2018 10:30
 Operator : JU/SJ
 Sample : PB111850BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB111850BL

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_F\METHODS\8270-BF080818.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	2.401	7	11	30	rVB2	143617	318829	3.08%	0.422%
2	5.260	491	497	506	rBV	1075141	1506421	14.54%	1.996%
3	5.642	556	562	565	rBV	7133060	7394553	71.39%	9.798%
4	6.630	723	730	733	rBV	7132584	7756946	74.89%	10.278%
5	6.783	751	756	759	rBV	7631772	7563606	73.02%	10.022%
6	7.013	791	795	798	rBV	2062102	1611042	15.55%	2.135%
7	7.172	817	822	825	rBV	6386572	5835837	56.34%	7.733%
8	7.572	885	890	893	rBV	4822883	5024198	48.51%	6.657%
9	8.295	1008	1013	1016	rBV	2334908	2018578	19.49%	2.675%
10	9.371	1190	1196	1199	rBV	8755245	8847815	85.42%	11.724%
11	10.060	1307	1313	1317	rBV	2603409	2347261	22.66%	3.110%
12	10.854	1441	1448	1451	rBV	5795507	5651600	54.56%	7.489%
13	11.554	1562	1567	1571	rBV	3006568	2585185	24.96%	3.426%
14	13.148	1828	1838	1841	rBV	10022525	10357941	100.00%	13.725%
15	14.206	2014	2018	2022	rBV	2918234	2793550	26.97%	3.702%
16	14.989	2146	2151	2158	rBV	193182	218126	2.11%	0.289%
17	15.359	2209	2214	2225	rVB	276227	372365	3.59%	0.493%
18	15.771	2277	2284	2292	rBV	1947772	2721927	26.28%	3.607%
19	16.253	2360	2366	2373	rBV	198244	326814	3.16%	0.433%
20	16.818	2456	2462	2472	rBV2	97282	215997	2.09%	0.286%

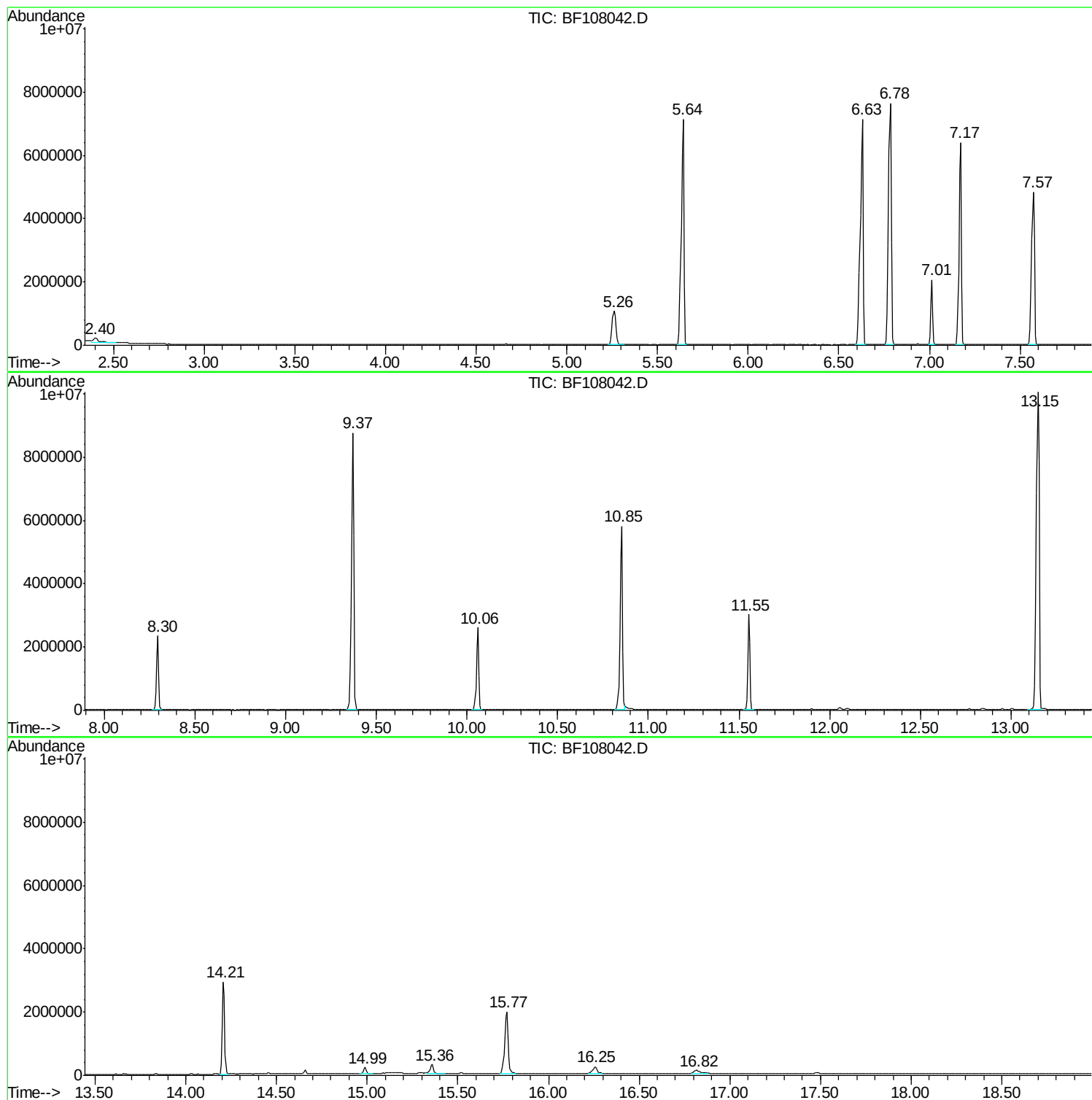
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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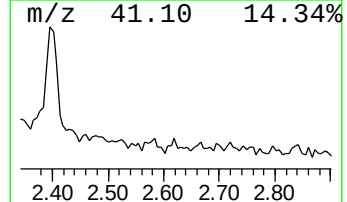
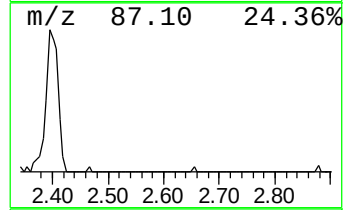
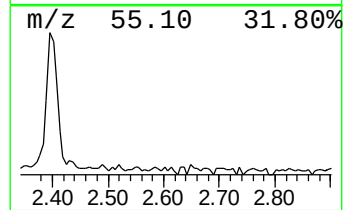
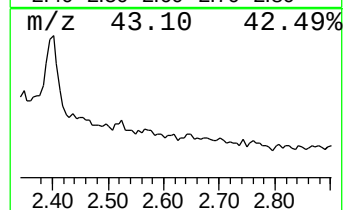
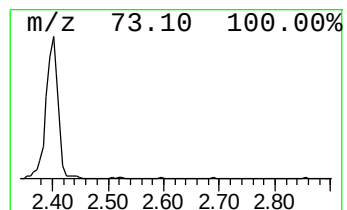
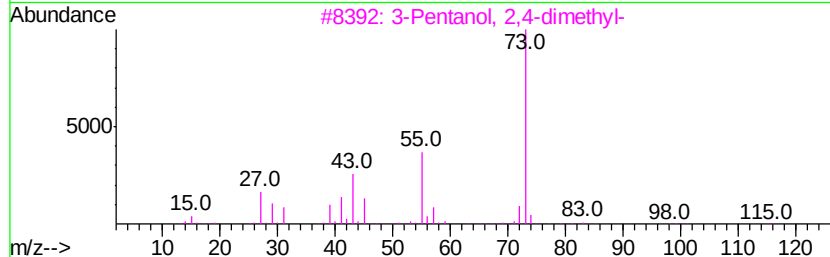
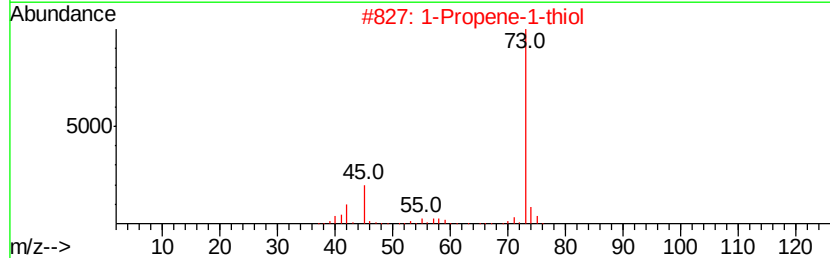
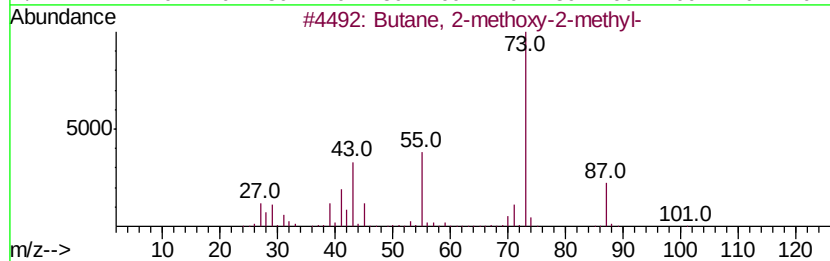
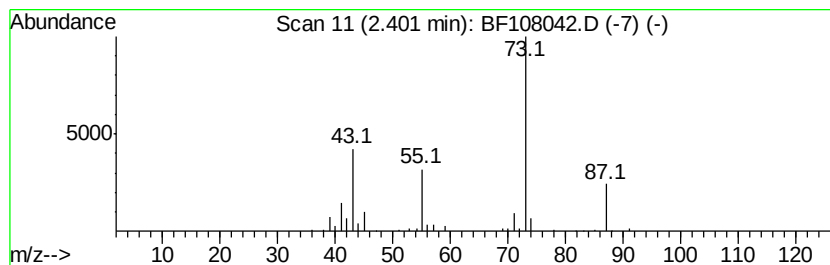
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	3.96 ng	318829	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		1-Propene-1-thiol	74	C3H6S	000925-89-3	49
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25



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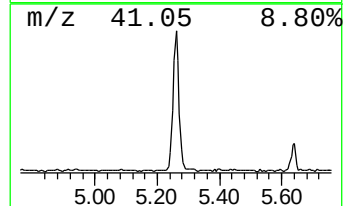
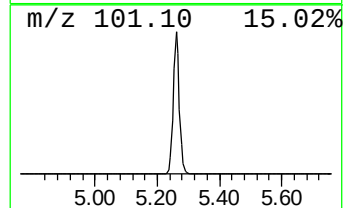
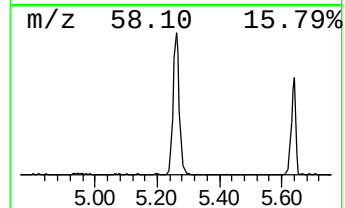
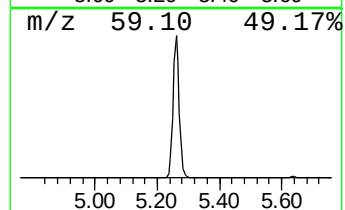
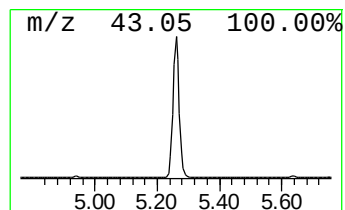
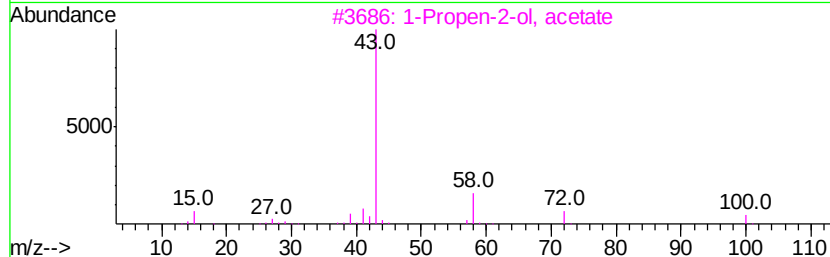
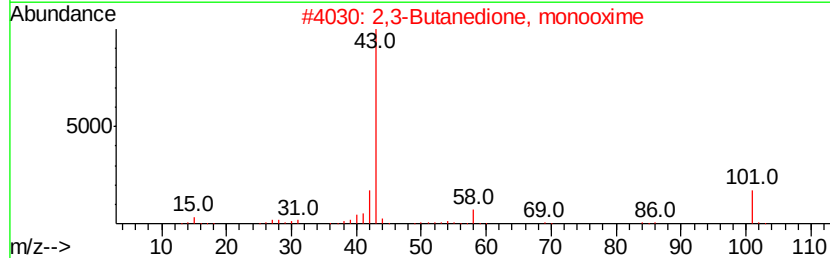
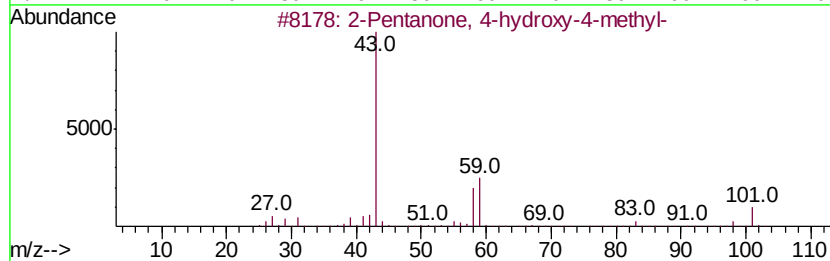
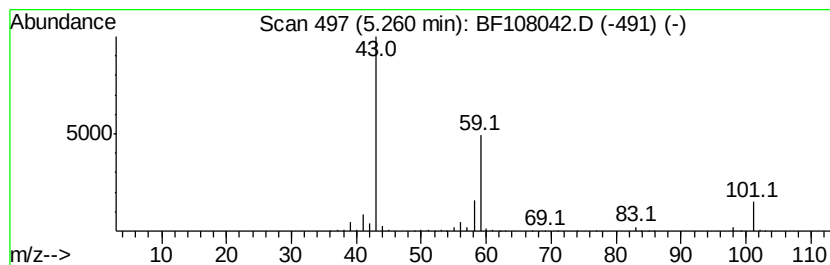
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	18.70 ng	1506420	1,4-Dichlorobenzene-d4	7.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9	
5	Allyl acetate	100	C5H8O2	000591-87-7	9	



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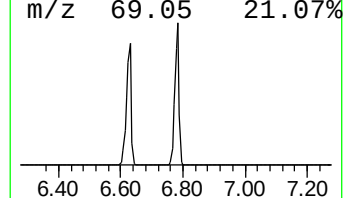
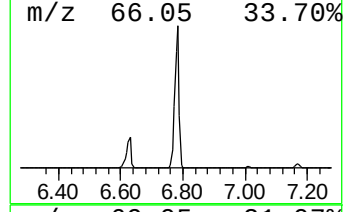
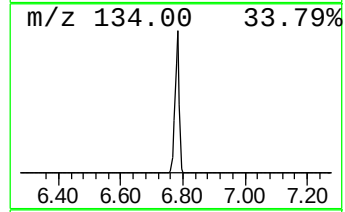
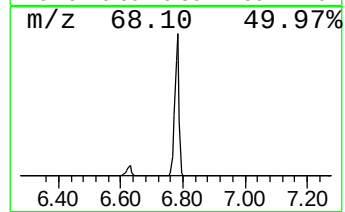
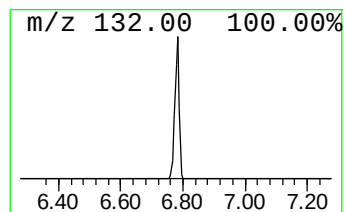
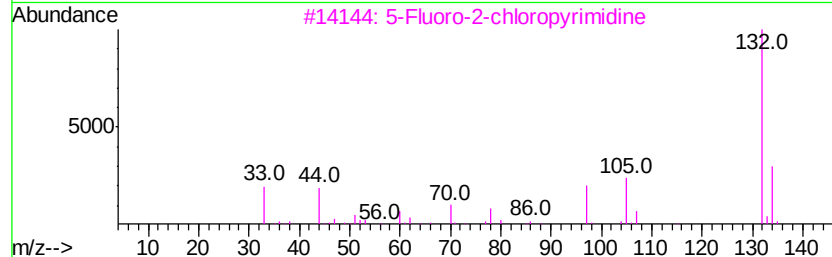
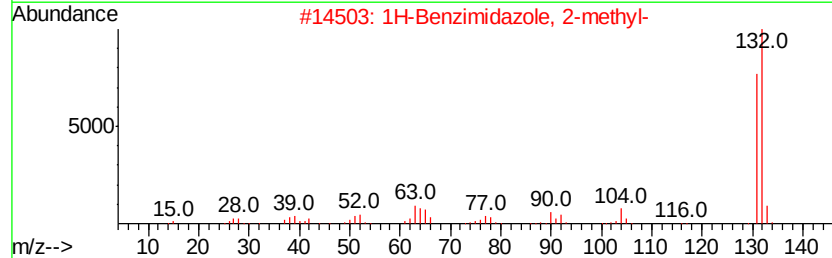
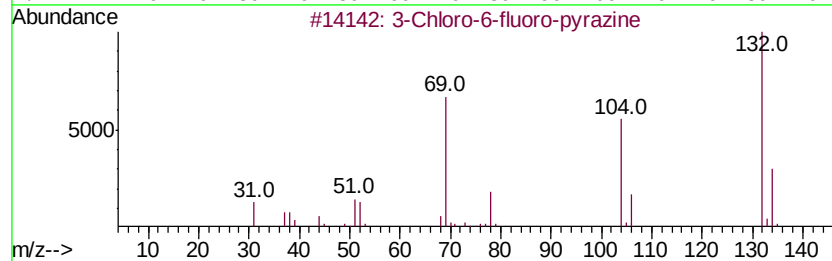
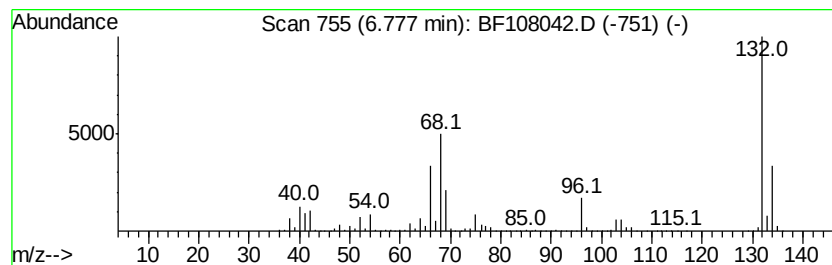
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Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	93.90 ng	7563610	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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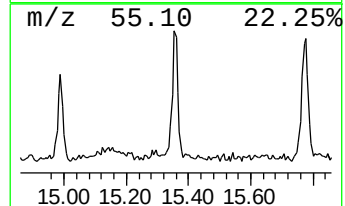
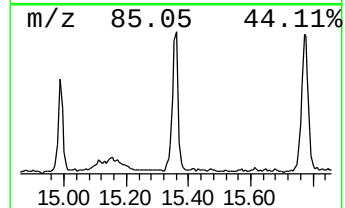
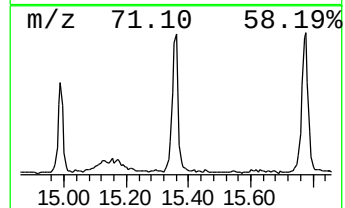
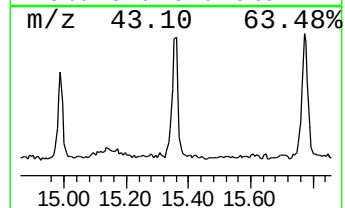
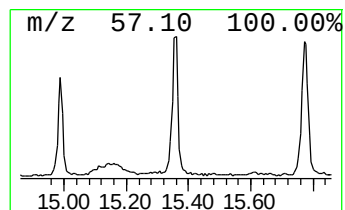
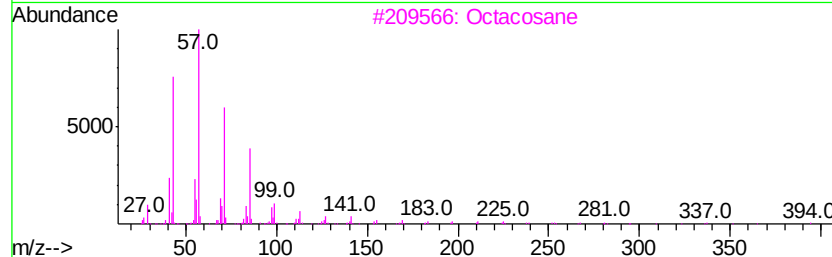
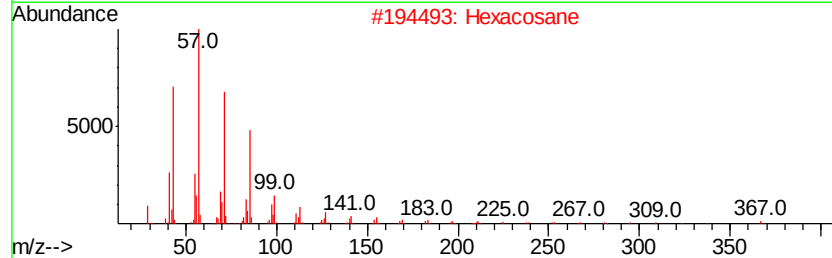
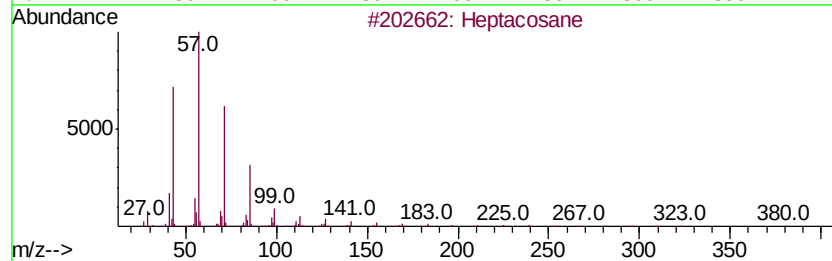
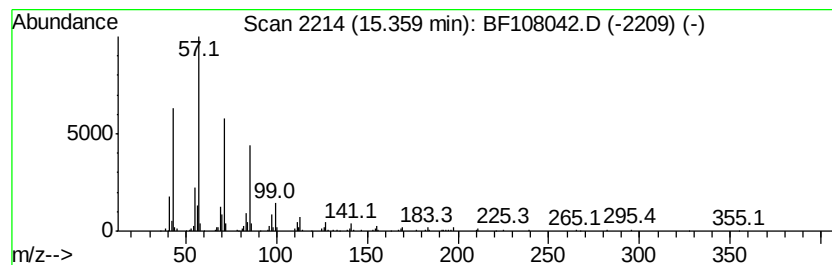
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.74 ng	372365	Perylene-d12	15.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Octacosane		394	C28H58	000630-02-4	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Octadecane		254	C18H38	000593-45-3	87



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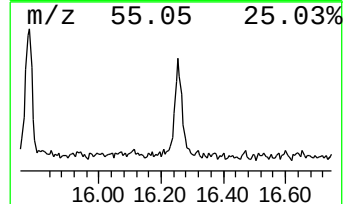
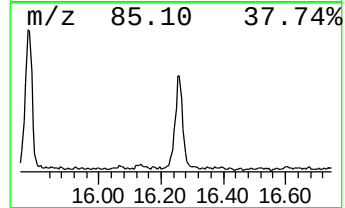
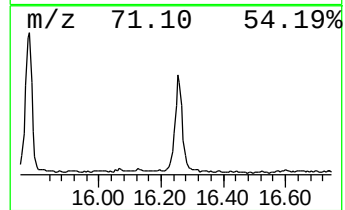
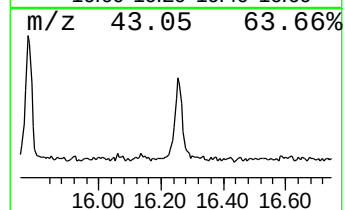
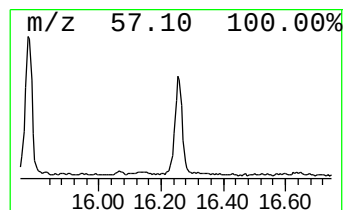
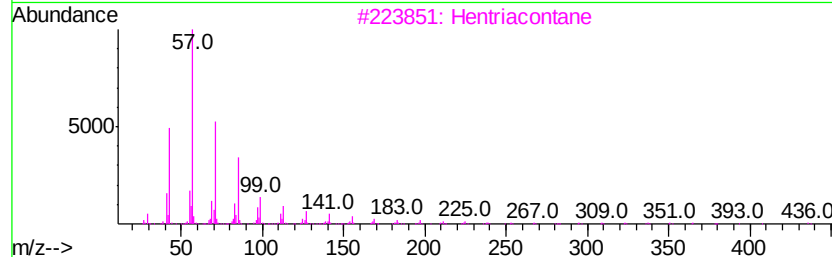
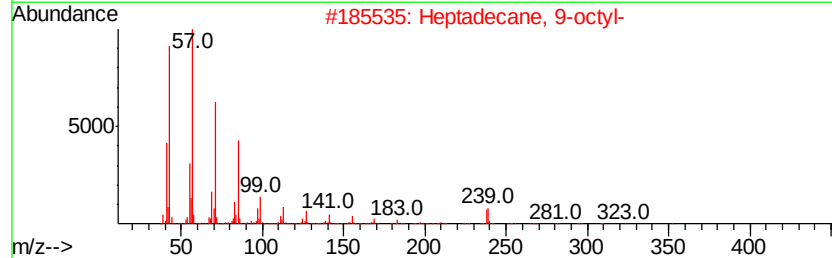
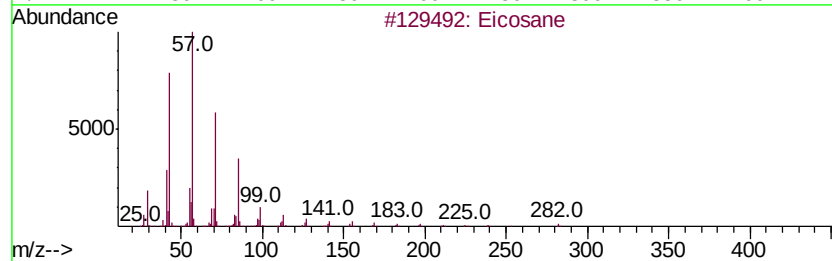
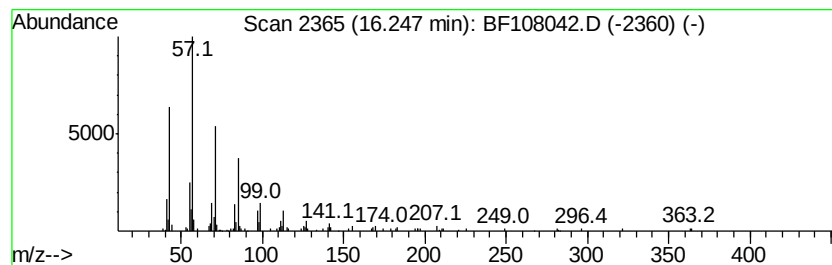
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.40 ng	326814	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		Hentriacontane	437	C31H64	000630-04-6	87
4		Pentacosane	352	C25H52	000629-99-2	87
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.40	4.0	ng	318829	1	7.01	1611040	20.0
2-Pentanone, 4-hy...	5.26	18.7	ng	1506420	1	7.01	1611040	20.0
unknown6.78	6.78	93.9	ng	7563610	1	7.01	1611040	20.0
Heptacosane	15.36	2.7	ng	372365	6	15.77	2721930	20.0
Eicosane	16.25	2.4	ng	326814	6	15.77	2721930	20.0