

Data Path : U:\HPCHEM1\BNA_F\DATA\BF082217\
 Data File : BF097979.D
 Acq On : 23 Aug 2017 3:14
 Operator : SJ/JU
 Sample : I4914-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 289-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	3.134	176	178	187	rBV	47975	87584	2.54%	0.307%
2	4.951	483	487	498	rVB	190334	277265	8.05%	0.972%
3	5.363	552	557	560	rBV	3085182	3206730	93.14%	11.245%
4	6.387	725	731	737	rBV	2832925	3442824	100.00%	12.073%
5	6.522	749	754	757	rBV	3178297	3151347	91.53%	11.050%
6	6.745	789	792	796	rBV	898227	805432	23.39%	2.824%
7	6.904	815	819	823	rBV	2612702	2519535	73.18%	8.835%
8	7.316	883	889	892	rBV	2047278	2083999	60.53%	7.308%
9	8.034	1006	1011	1014	rBV	1137232	1009742	29.33%	3.541%
10	9.110	1188	1194	1197	rBV	3454177	3116299	90.52%	10.928%
11	9.498	1256	1260	1264	rBV	423420	391941	11.38%	1.374%
12	9.781	1304	1308	1312	rBV	1028546	955188	27.74%	3.349%
13	10.569	1438	1442	1450	rBV	1507744	1372202	39.86%	4.812%
14	10.692	1460	1463	1472	rBV	67750	75170	2.18%	0.264%
15	11.139	1536	1539	1542	rBV	41816	35613	1.03%	0.125%
16	11.263	1556	1560	1563	rBV	946407	812994	23.61%	2.851%
17	11.286	1563	1564	1567	rVB	100181	60553	1.76%	0.212%
18	12.474	1763	1766	1769	rBV	150736	135517	3.94%	0.475%
19	12.698	1798	1804	1807	rBV	136612	154266	4.48%	0.541%
20	12.851	1826	1830	1833	rBV	2279204	2138781	62.12%	7.500%
21	13.392	1919	1922	1927	rBV2	33884	37335	1.08%	0.131%
22	13.751	1979	1983	1988	rBV2	109054	124449	3.61%	0.436%
23	13.892	2003	2007	2011	rBV2	1033371	1268378	36.84%	4.448%
24	13.921	2011	2012	2015	rVB	70808	40210	1.17%	0.141%
25	14.004	2023	2026	2030	rVB	60231	54021	1.57%	0.189%
26	14.386	2088	2091	2093	rBV	39542	45706	1.33%	0.160%
27	14.533	2113	2116	2120	rBV	93096	107822	3.13%	0.378%
28	14.745	2150	2152	2159	rVB4	33871	43299	1.26%	0.152%
29	14.816	2162	2164	2167	rVB3	43660	36309	1.05%	0.127%
30	14.910	2177	2180	2183	rBV	53975	67363	1.96%	0.236%
31	15.198	2226	2229	2233	rBV	34247	40149	1.17%	0.141%
32	15.257	2236	2239	2242	rBV	41481	39831	1.16%	0.140%
33	15.321	2245	2250	2254	rBV	507628	577424	16.77%	2.025%
34	15.774	2324	2327	2332	rVB2	51747	71532	2.08%	0.251%

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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

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35	16.251	2405	2408	2413	rVB	40550	59431	1.73%	0.208%
36	16.809	2500	2503	2510	rVB2	43792	71588	2.08%	0.251%

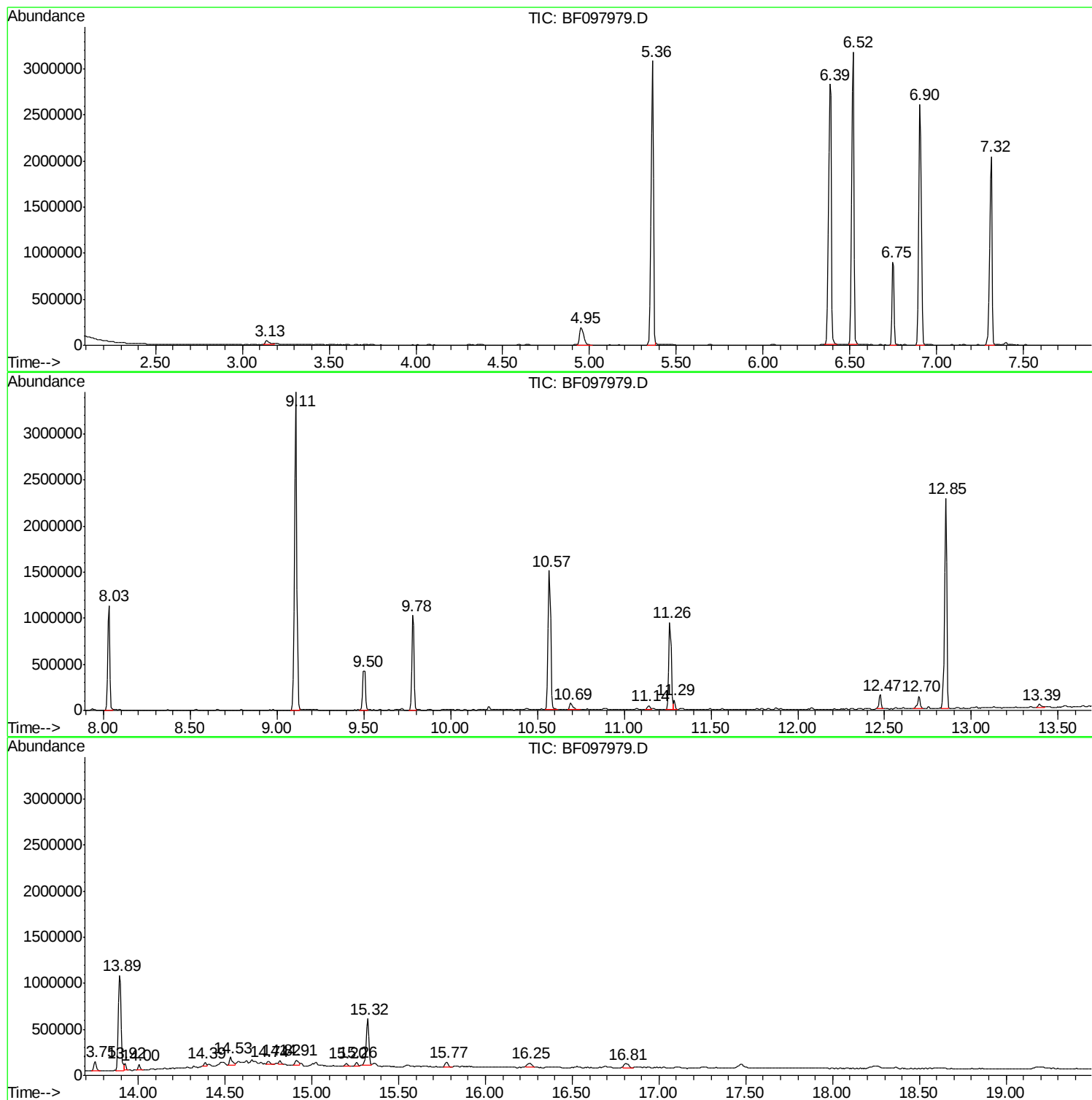
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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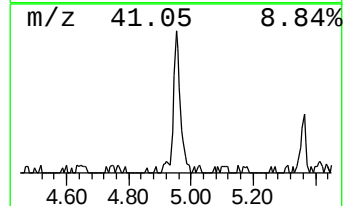
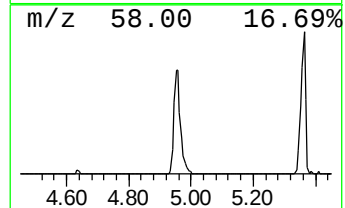
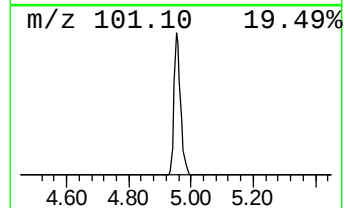
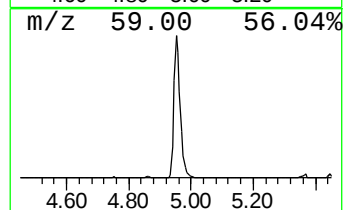
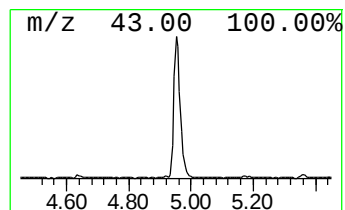
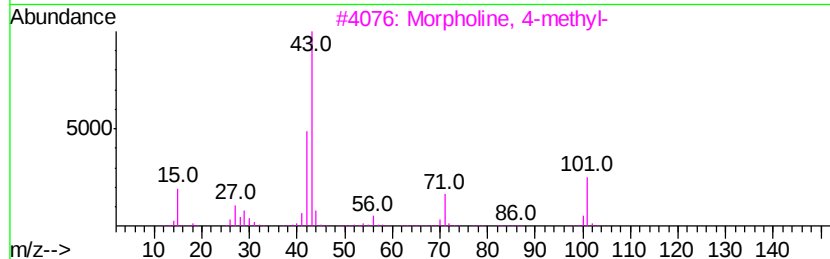
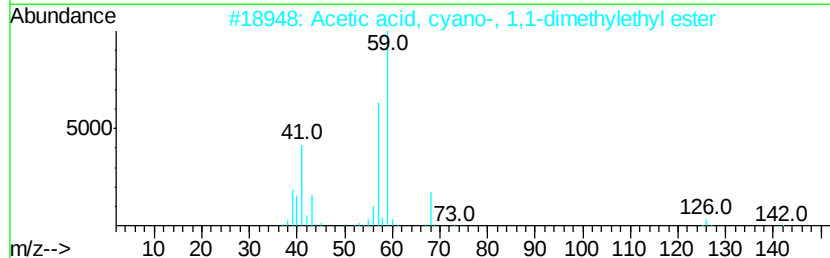
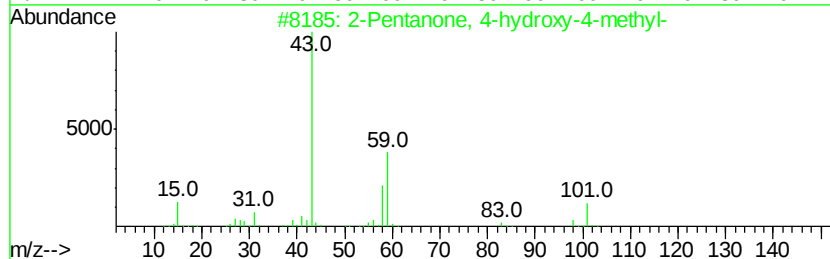
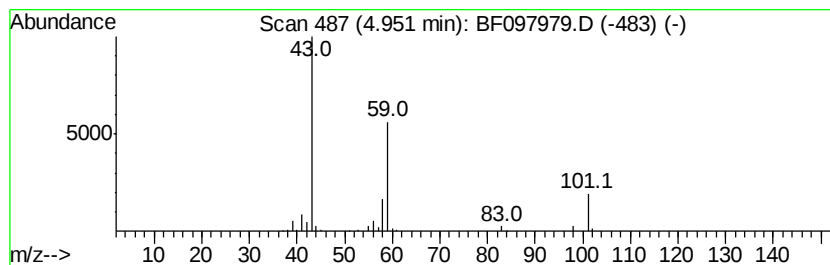
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	6.88 ng	277265	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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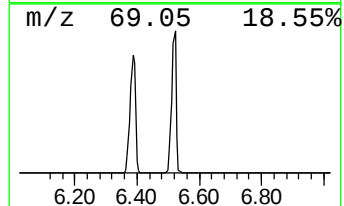
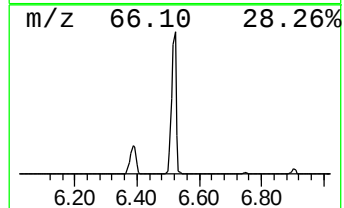
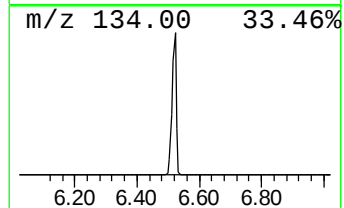
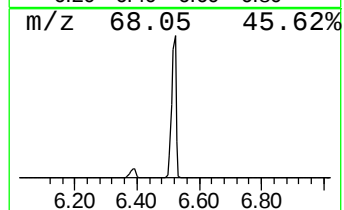
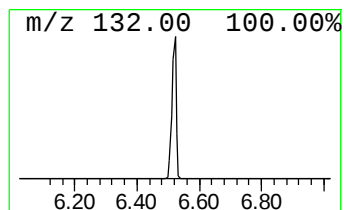
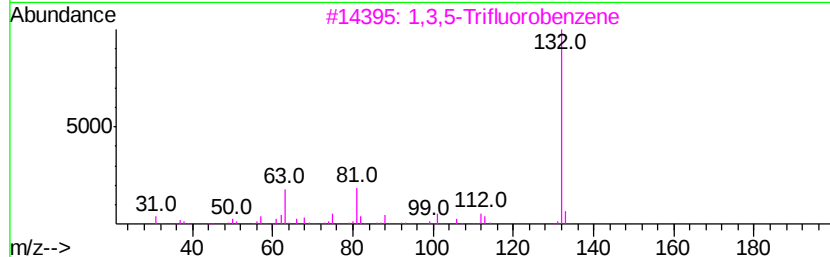
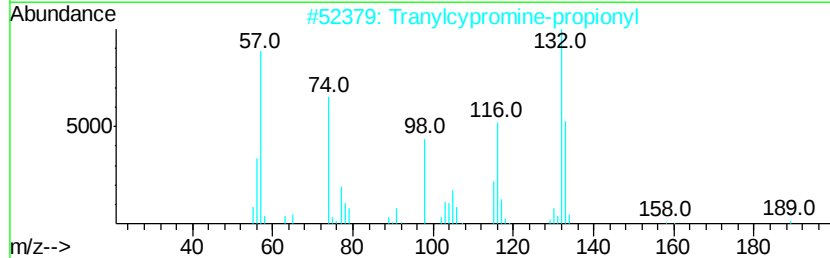
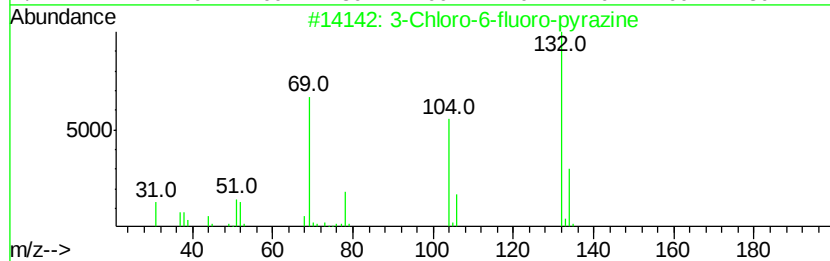
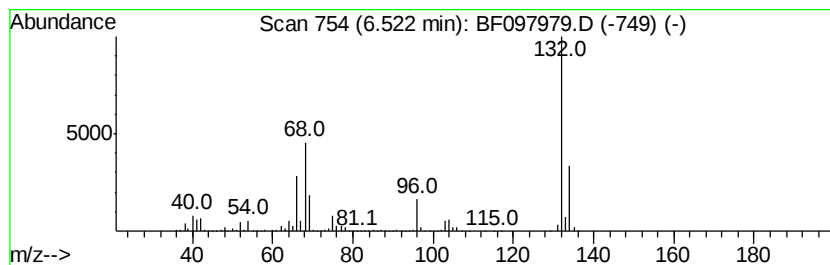
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	78.25 ng	3151350	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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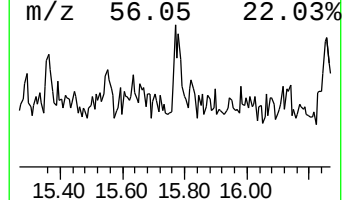
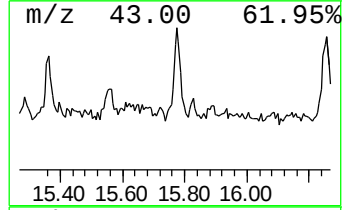
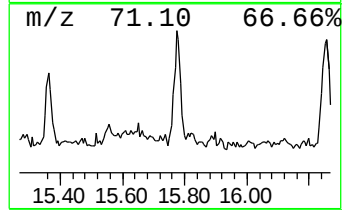
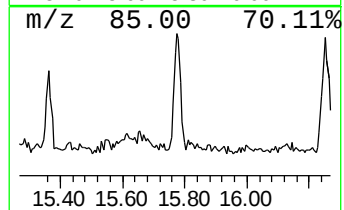
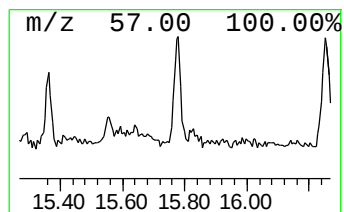
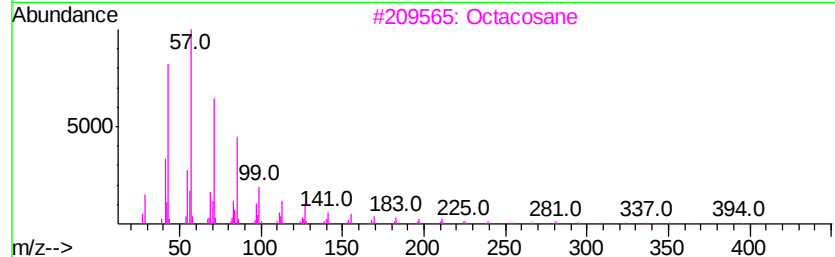
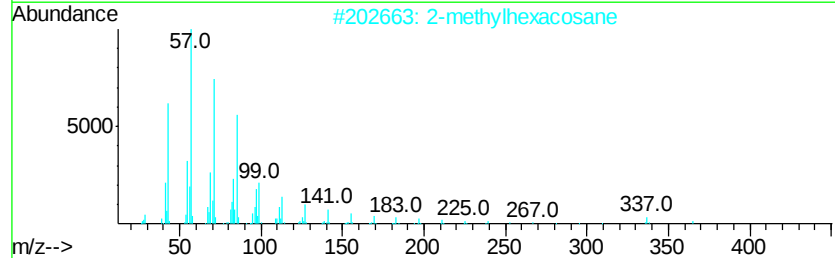
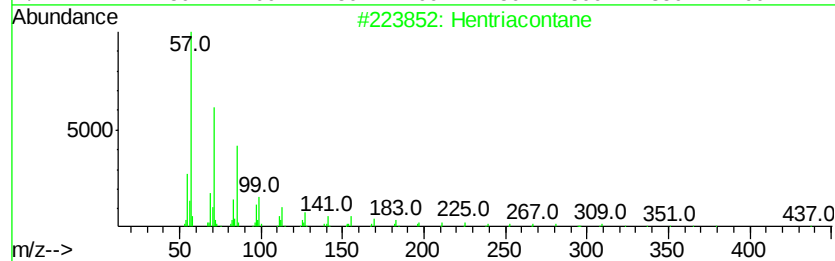
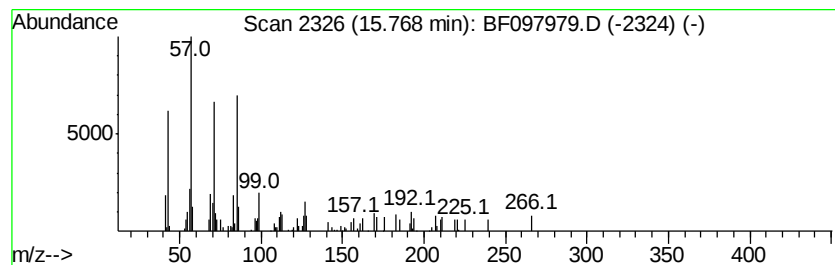
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.48 ng	71532	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	74
2		2-methylhexacosane	380	C27H56	1000376-72-7	72
3		Octacosane	394	C28H58	000630-02-4	72
4		2-methyloctacosane	408	C29H60	1000376-72-8	72
5		2-methyltetracosane	352	C25H52	1000376-72-6	72



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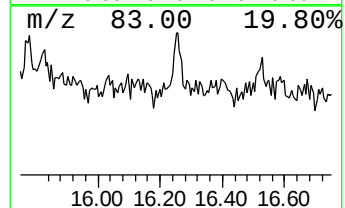
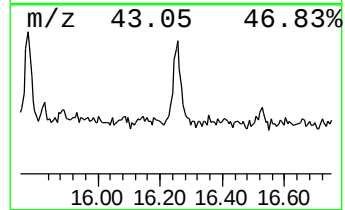
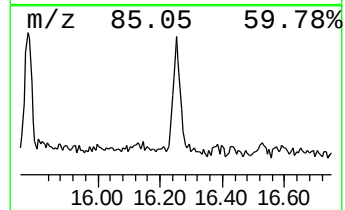
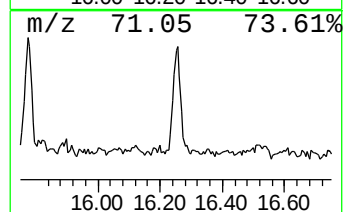
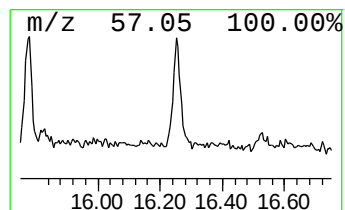
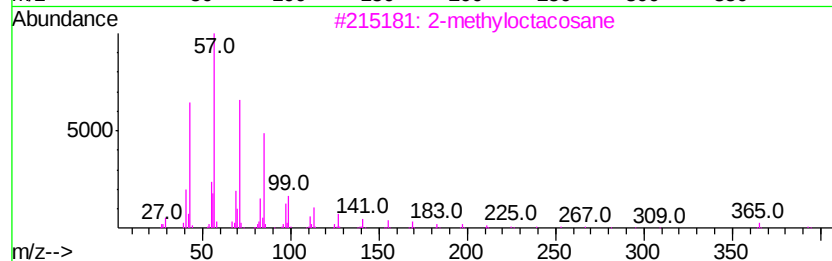
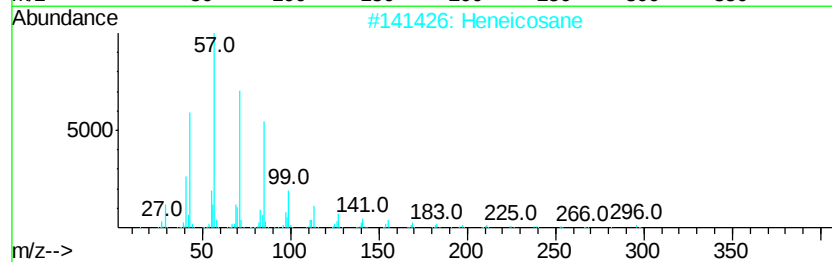
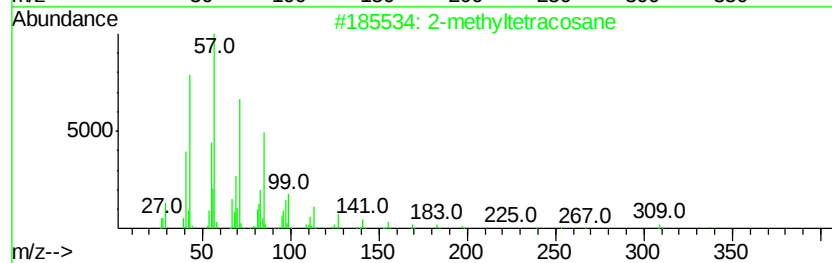
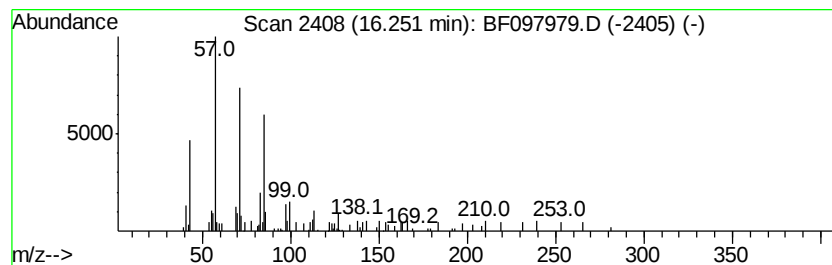
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-methyltetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.06 ng	59431	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyltetracosane	352	C25H52	1000376-72-6	86
2		Heneicosane	296	C21H44	000629-94-7	72
3		2-methyloctacosane	408	C29H60	1000376-72-8	64
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5		Nonacosane	408	C29H60	000630-03-5	64



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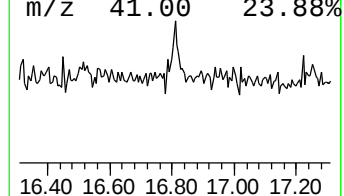
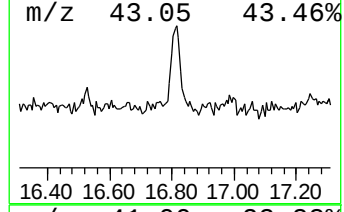
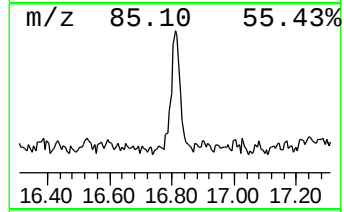
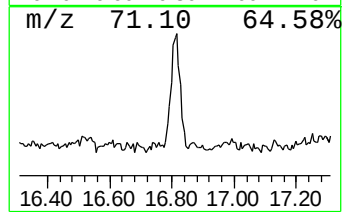
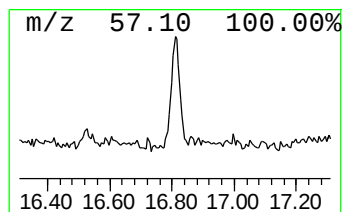
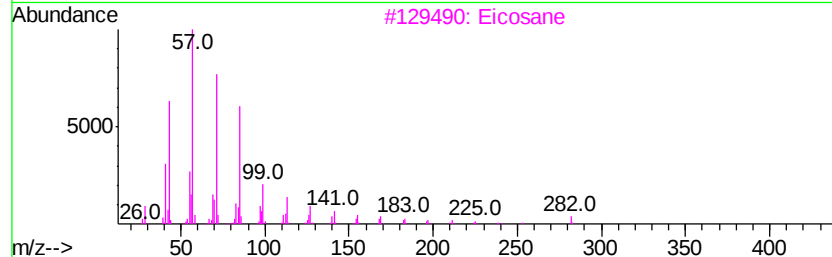
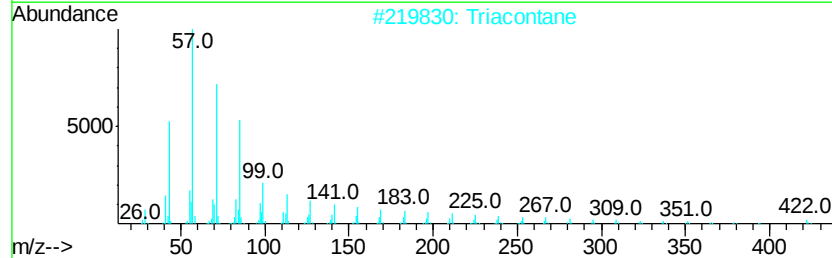
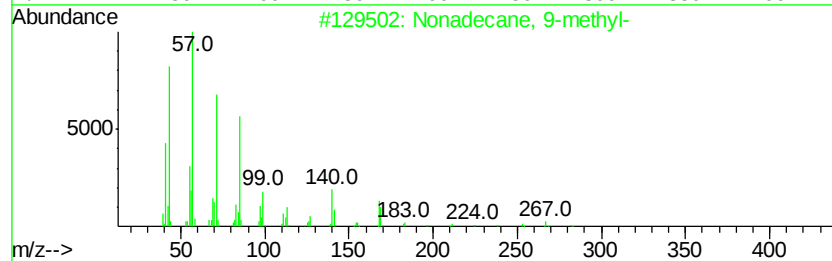
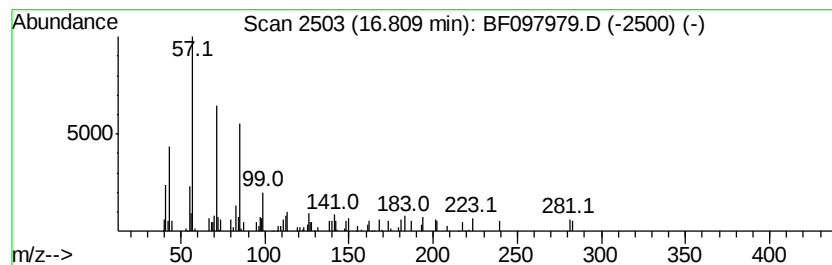
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Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	2.48 ng	71588	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64
2		Triacontane	422	C30H62	000638-68-6	64
3		Eicosane	282	C20H42	000112-95-8	64
4		Nonadecane	268	C19H40	000629-92-5	53
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50



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289-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.95	6.9	ng	277265	1	6.75	805432	20.0
unknown6.52	6.52	78.3	ng	3151350	1	6.75	805432	20.0
Hentriacontane	15.77	2.5	ng	71532	6	15.32	577424	20.0
2-methyltetracosane	16.25	2.1	ng	59431	6	15.32	577424	20.0
Nonadecane, 9-met...	16.81	2.5	ng	71588	6	15.32	577424	20.0