

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
 Data File : BF134399.D
 Acq On : 21 Jul 2023 13:58
 Operator : CG\JU
 Sample : 03638-31
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP7

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	504	507	516	rBV	52680	62962	5.46%	0.689%
2	5.469	571	575	593	rBV	971788	904139	78.44%	9.893%
3	6.475	742	746	765	rBV	1092497	953417	82.71%	10.433%
4	6.834	804	807	821	rBV	415059	356708	30.95%	3.903%
5	7.398	899	903	915	rBV	716525	581448	50.44%	6.362%
6	8.116	1021	1025	1042	rBV	575458	471918	40.94%	5.164%
7	9.192	1204	1208	1211	rBV	1443659	1136261	98.57%	12.433%
8	9.875	1320	1324	1327	rBV	572097	510719	44.31%	5.588%
9	10.669	1455	1459	1470	rBV	784294	772647	67.03%	8.455%
10	11.369	1574	1578	1581	rBV	645919	546433	47.40%	5.979%
11	11.392	1581	1582	1586	rVB	40443	23419	2.03%	0.256%
12	11.874	1659	1664	1665	rBV3	9783	14230	1.23%	0.156%
13	11.898	1665	1668	1680	rVB3	112987	132264	11.47%	1.447%
14	12.592	1782	1786	1792	rBV	85086	89095	7.73%	0.975%
15	12.686	1800	1802	1806	rBV2	18972	21692	1.88%	0.237%
16	12.821	1819	1825	1828	rBV	76939	72133	6.26%	0.789%
17	12.963	1845	1849	1853	rBV	1388198	1152715	100.00%	12.613%
18	13.533	1942	1946	1949	rBV3	19935	20775	1.80%	0.227%
19	13.868	2000	2003	2008	rBV2	30242	29475	2.56%	0.323%
20	13.933	2008	2014	2023	rVV9	25934	87032	7.55%	0.952%
21	14.033	2026	2031	2034	rVV	419817	460461	39.95%	5.039%
22	14.057	2034	2035	2041	rVB	39874	29063	2.52%	0.318%
23	14.186	2054	2057	2065	rBV2	27074	28278	2.45%	0.309%
24	14.492	2107	2109	2115	rVB2	27578	28108	2.44%	0.308%
25	14.810	2160	2163	2165	rBV	16271	15451	1.34%	0.169%
26	14.957	2185	2188	2193	rBV2	20054	24309	2.11%	0.266%
27	15.098	2207	2212	2215	rBV	23693	37551	3.26%	0.411%
28	15.157	2219	2222	2226	rVB2	22472	25434	2.21%	0.278%
29	15.404	2261	2264	2270	rBV	13627	17724	1.54%	0.194%
30	15.468	2272	2275	2282	rVB2	17063	24042	2.09%	0.263%
31	15.539	2282	2287	2294	rBV	251947	342178	29.68%	3.744%
32	16.004	2363	2366	2373	rBV3	14517	25849	2.24%	0.283%
33	16.545	2453	2458	2466	rBV3	7632	17244	1.50%	0.189%
34	17.086	2546	2550	2555	rVB4	9750	15484	1.34%	0.169%
35	17.221	2568	2573	2579	rVB7	44969	86602	7.51%	0.948%
36	17.556	2625	2630	2638	rVB5	8451	21554	1.87%	0.236%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

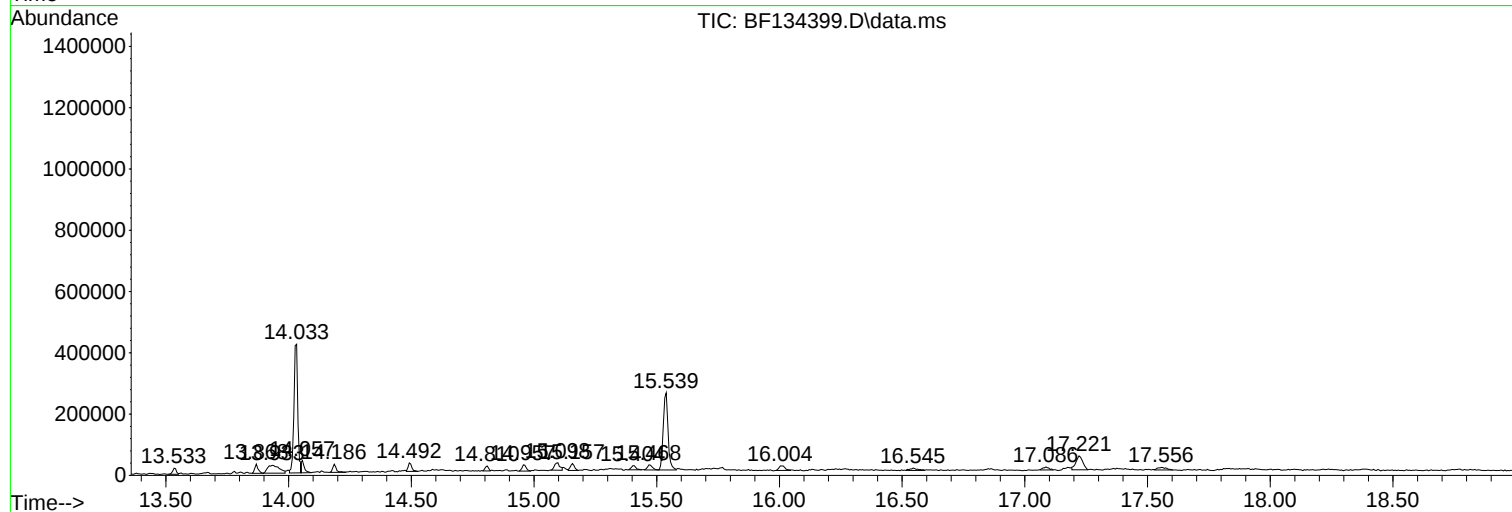
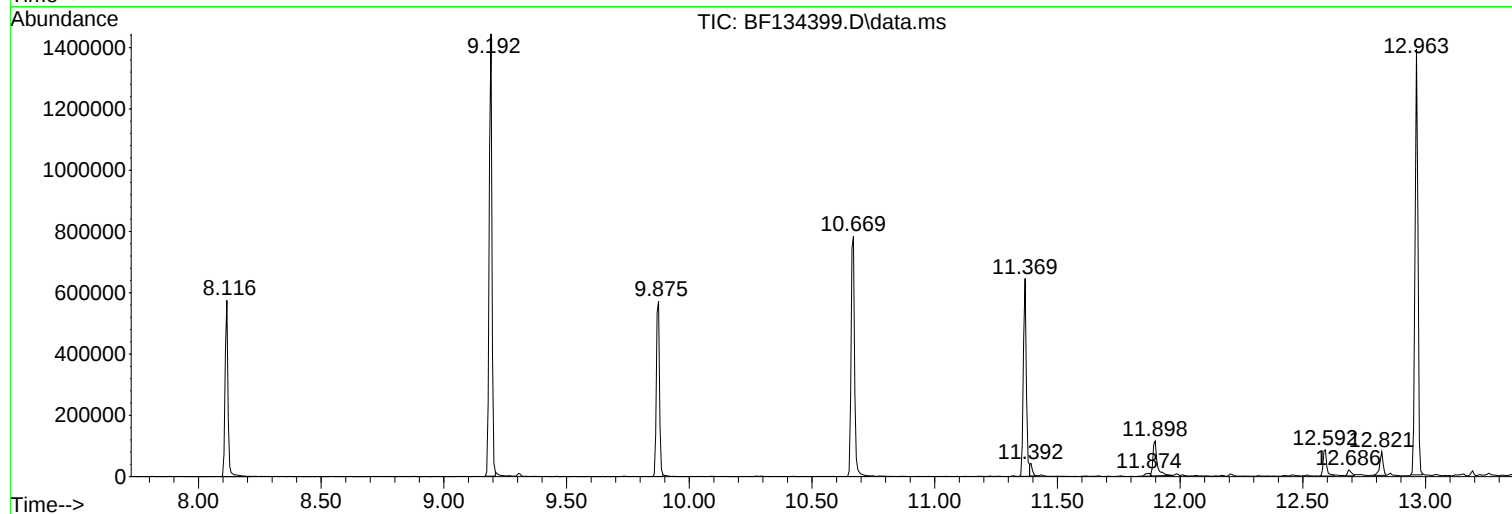
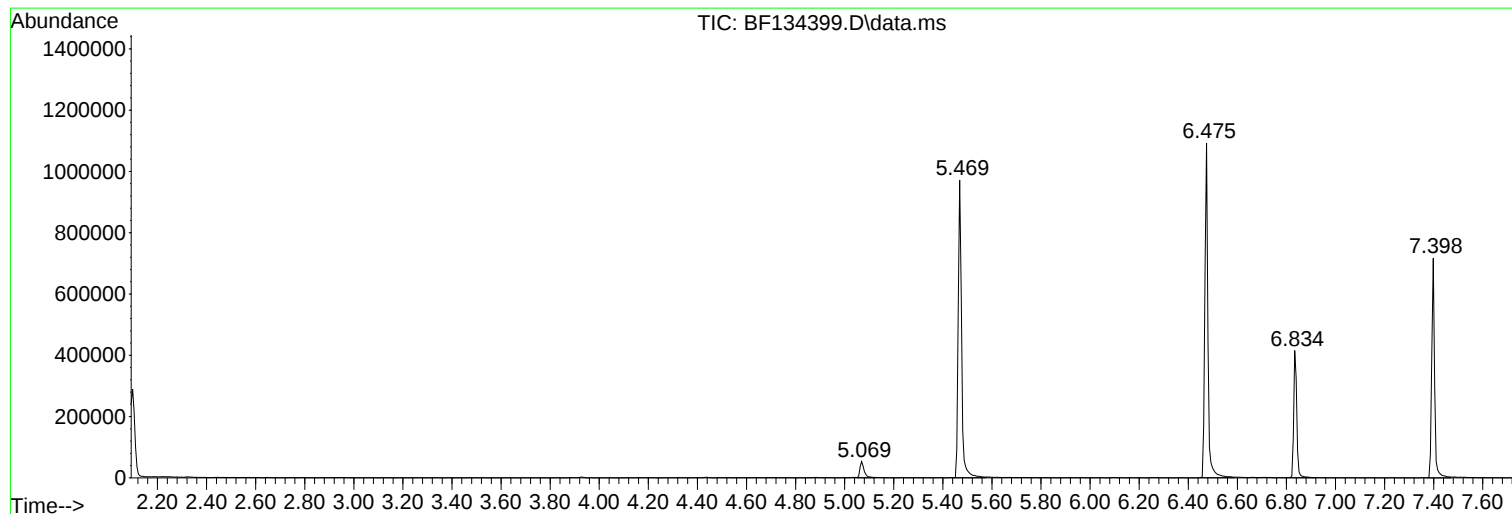
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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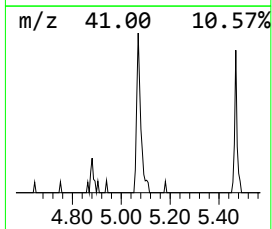
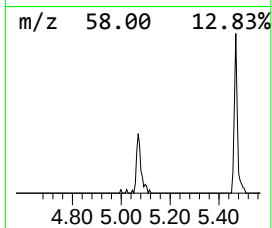
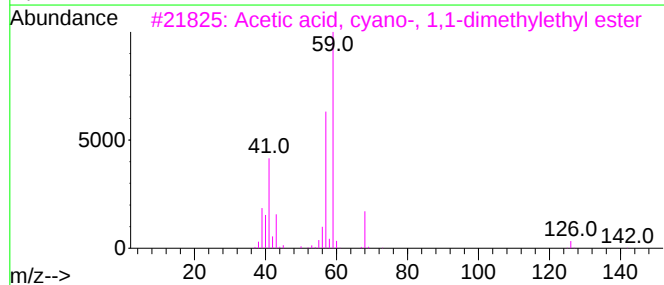
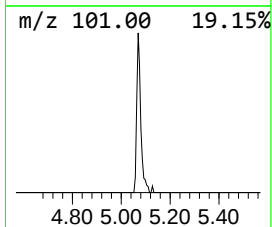
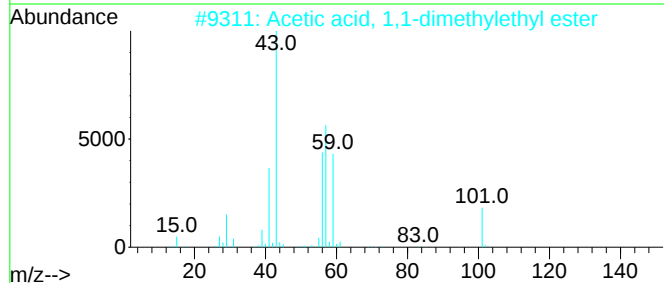
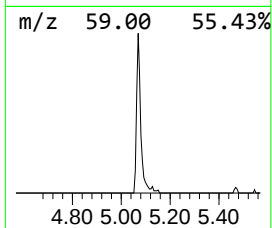
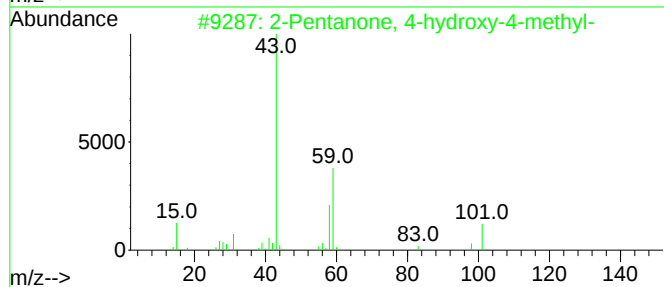
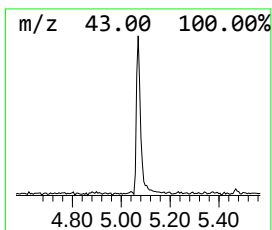
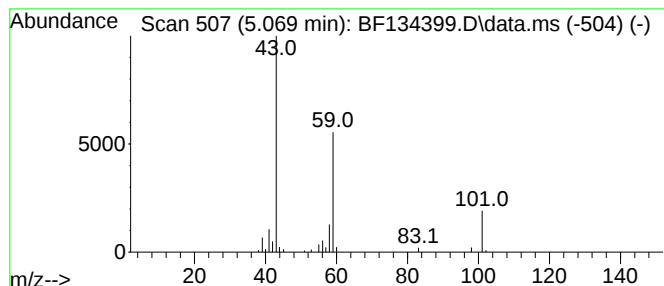
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	3.53 ng	62962	1,4-Dichlorobenzene-d4	6.834

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	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		



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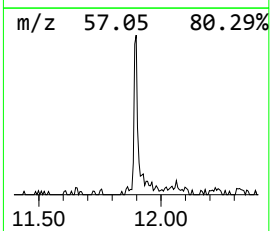
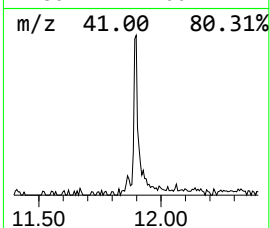
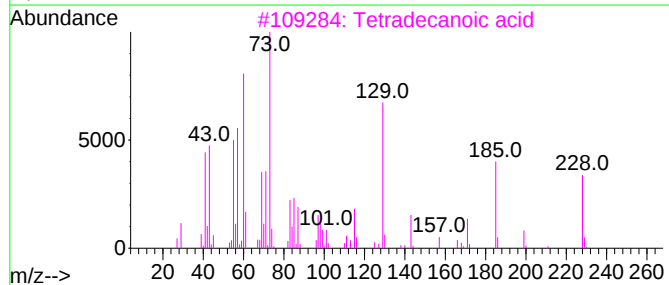
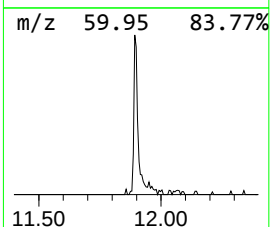
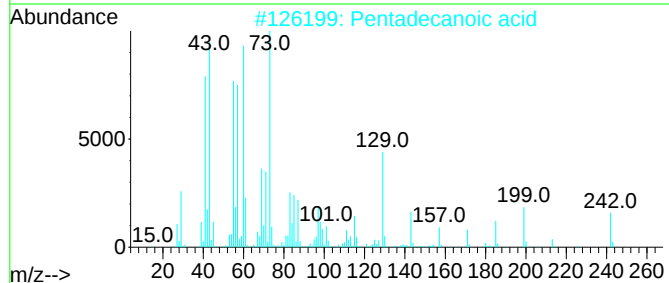
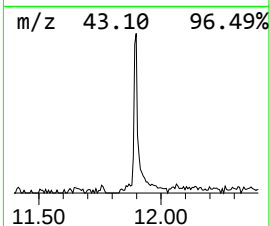
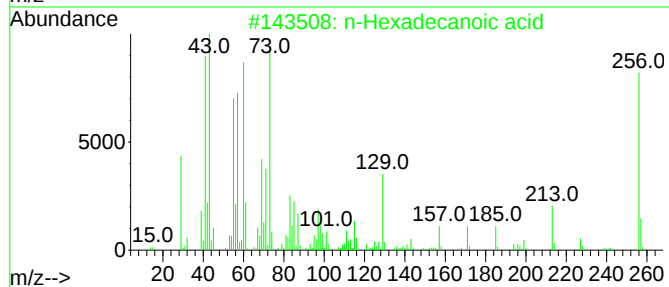
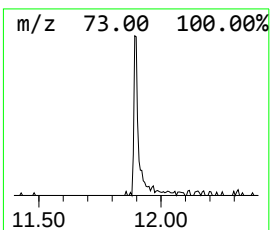
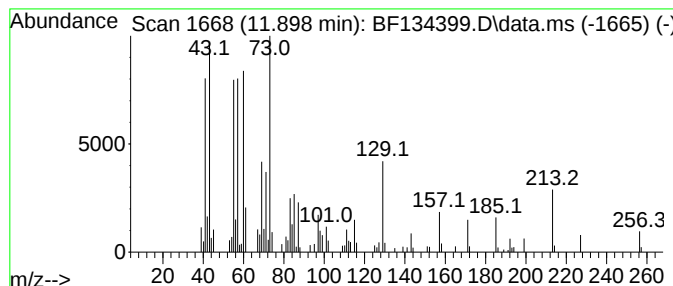
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	4.84 ng	132264	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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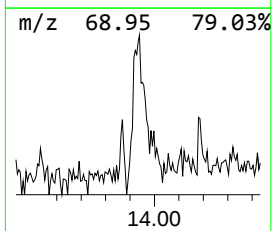
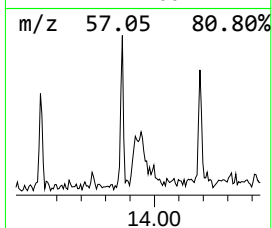
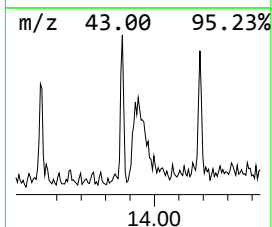
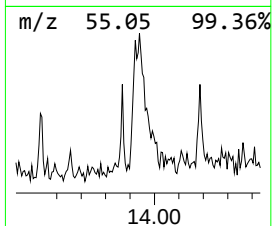
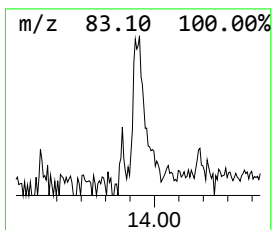
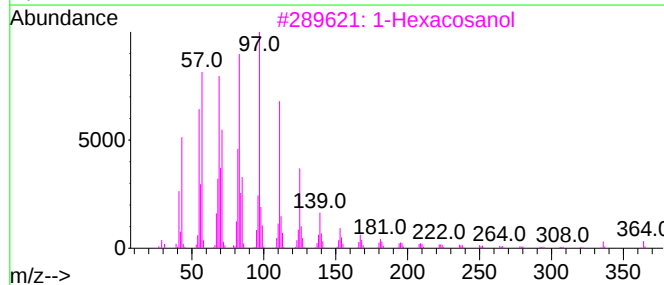
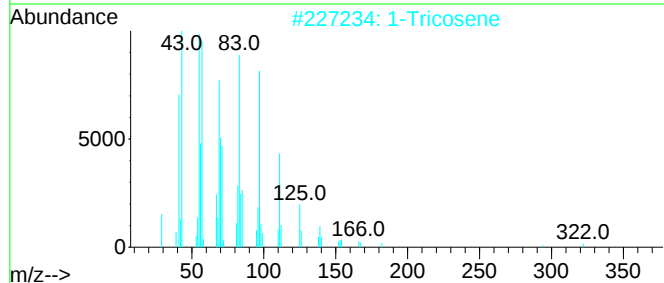
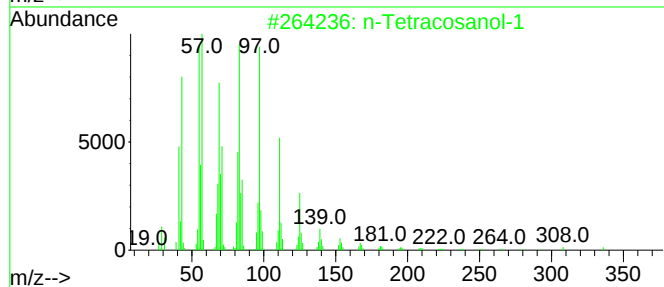
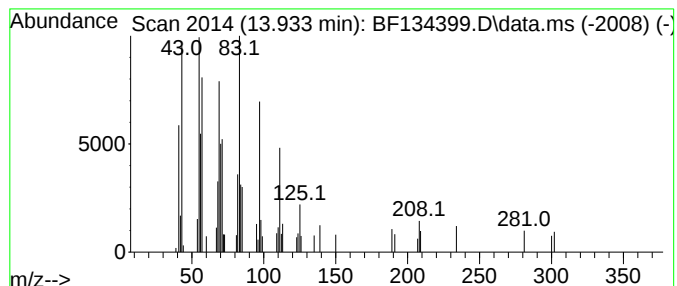
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	3.78 ng	87032	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2		1-Tricosene	322	C23H46	018835-32-0	87
3		1-Hexacosanol	382	C26H54O	000506-52-5	83
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83



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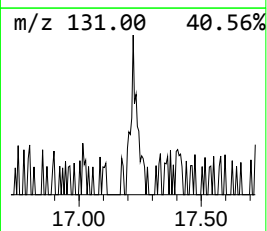
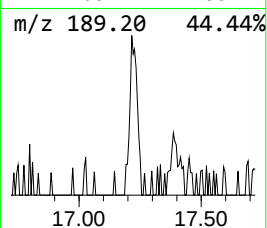
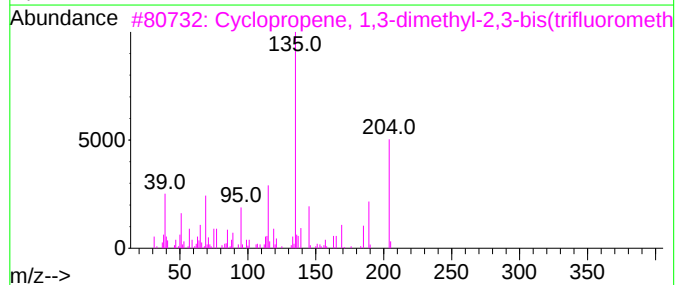
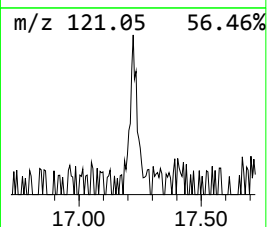
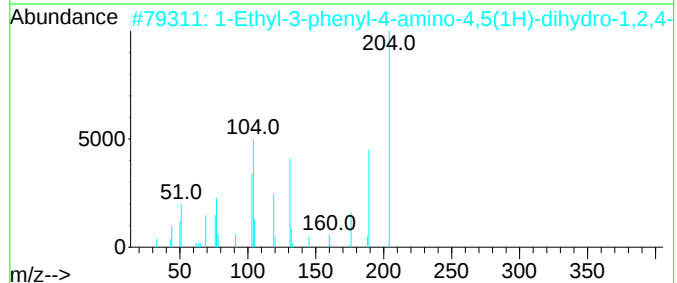
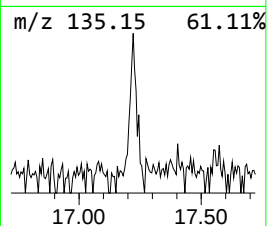
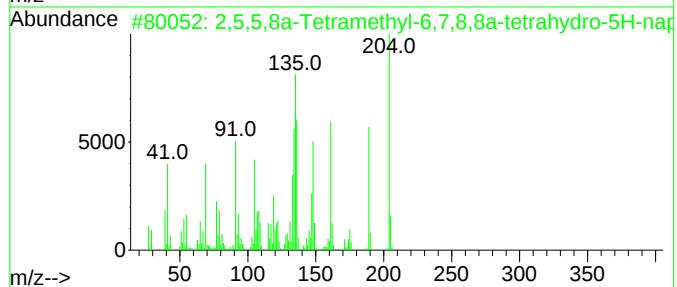
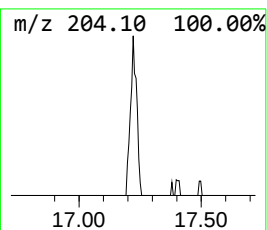
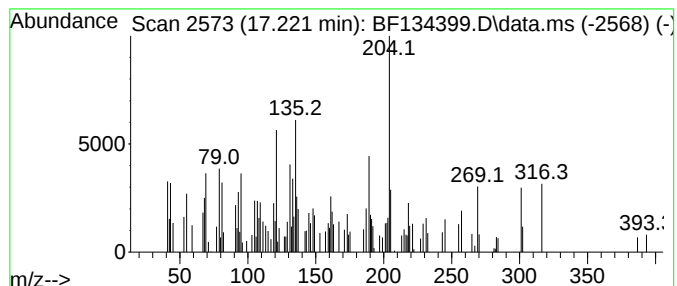
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown17.221 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.221	5.06 ng	86602	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46		
2	1-Ethyl-3-phenyl-4-amino-4,5(1H)...	204	C10H12N4O	073316-60-6	43		
3	Cyclopropene, 1,3-dimethyl-2,3-b...	204	C7H6F6	054932-73-9	38		
4	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	27		
5	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	27		



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.069	3.5	ng	62962	1	6.834	356708	20.0
n-Hexadecanoic ...	11.898	4.8	ng	132264	4	11.369	546433	20.0
n-Tetracosanol-1	13.933	3.8	ng	87032	5	14.033	460461	20.0
unknown17.221	17.221	5.1	ng	86602	6	15.539	342178	20.0