

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
 Data File : BF095966.D
 Acq On : 16 Jun 2017 20:50
 Operator : SJ/MA
 Sample : I3689-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BAYWAY-SWITCH-A

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-BF060517.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	4.510	493	497	513	rBV	38893	102842	7.18%	0.855%
2	5.216	614	617	656	rBV	464286	1123989	78.46%	9.349%
3	6.892	899	902	913	rBV	590834	1038248	72.47%	8.636%
4	6.981	913	917	940	rVB	810602	1411289	98.51%	11.738%
5	7.322	971	975	985	rBV	272794	377260	26.33%	3.138%
6	7.557	1010	1015	1030	rBV	680498	904450	63.13%	7.523%
7	8.239	1127	1131	1155	rBV	429142	685949	47.88%	5.705%
8	9.351	1316	1320	1339	rBV	371623	523700	36.56%	4.356%
9	11.127	1617	1622	1642	rBV	1093280	1432595	100.00%	11.915%
10	11.827	1738	1741	1752	rBV	78129	110389	7.71%	0.918%
11	12.168	1795	1799	1806	rBV2	426713	560121	39.10%	4.659%
12	13.027	1941	1945	1949	rBV	15756	18715	1.31%	0.156%
13	13.468	2015	2020	2036	rBV	461580	702752	49.05%	5.845%
14	13.798	2072	2076	2084	rBV	15453	22149	1.55%	0.184%
15	14.562	2202	2206	2211	rBV	393942	500750	34.95%	4.165%
16	14.604	2211	2213	2223	rVB	42481	66848	4.67%	0.556%
17	15.380	2341	2345	2349	rBV	13946	16166	1.13%	0.134%
18	15.427	2349	2353	2359	rVB	15388	20343	1.42%	0.169%
19	15.533	2367	2371	2376	rBV4	11853	20847	1.46%	0.173%
20	15.586	2376	2380	2389	rVB3	22079	35862	2.50%	0.298%
21	16.392	2513	2517	2523	rVB	73469	95329	6.65%	0.793%
22	16.698	2564	2569	2575	rBV	93348	122772	8.57%	1.021%
23	16.939	2606	2610	2618	rVB	915323	985054	68.76%	8.193%
24	17.309	2669	2673	2677	rBV2	10979	14904	1.04%	0.124%
25	18.203	2821	2825	2834	rBV2	28359	47616	3.32%	0.396%
26	18.286	2834	2839	2844	rBV	338777	426688	29.78%	3.549%
27	19.568	3053	3057	3060	rBV	43083	59141	4.13%	0.492%
28	19.591	3060	3061	3068	rVB2	17326	19765	1.38%	0.164%
29	19.850	3102	3105	3110	rVB	27910	30094	2.10%	0.250%
30	19.909	3110	3115	3119	rBV	43896	47189	3.29%	0.392%
31	19.956	3119	3123	3134	rBV	295661	407103	28.42%	3.386%
32	20.391	3193	3197	3201	rBV3	11376	16924	1.18%	0.141%
33	21.150	3320	3326	3338	rBV4	16385	42925	3.00%	0.357%
34	21.491	3378	3384	3389	rBV4	14969	32227	2.25%	0.268%

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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 >
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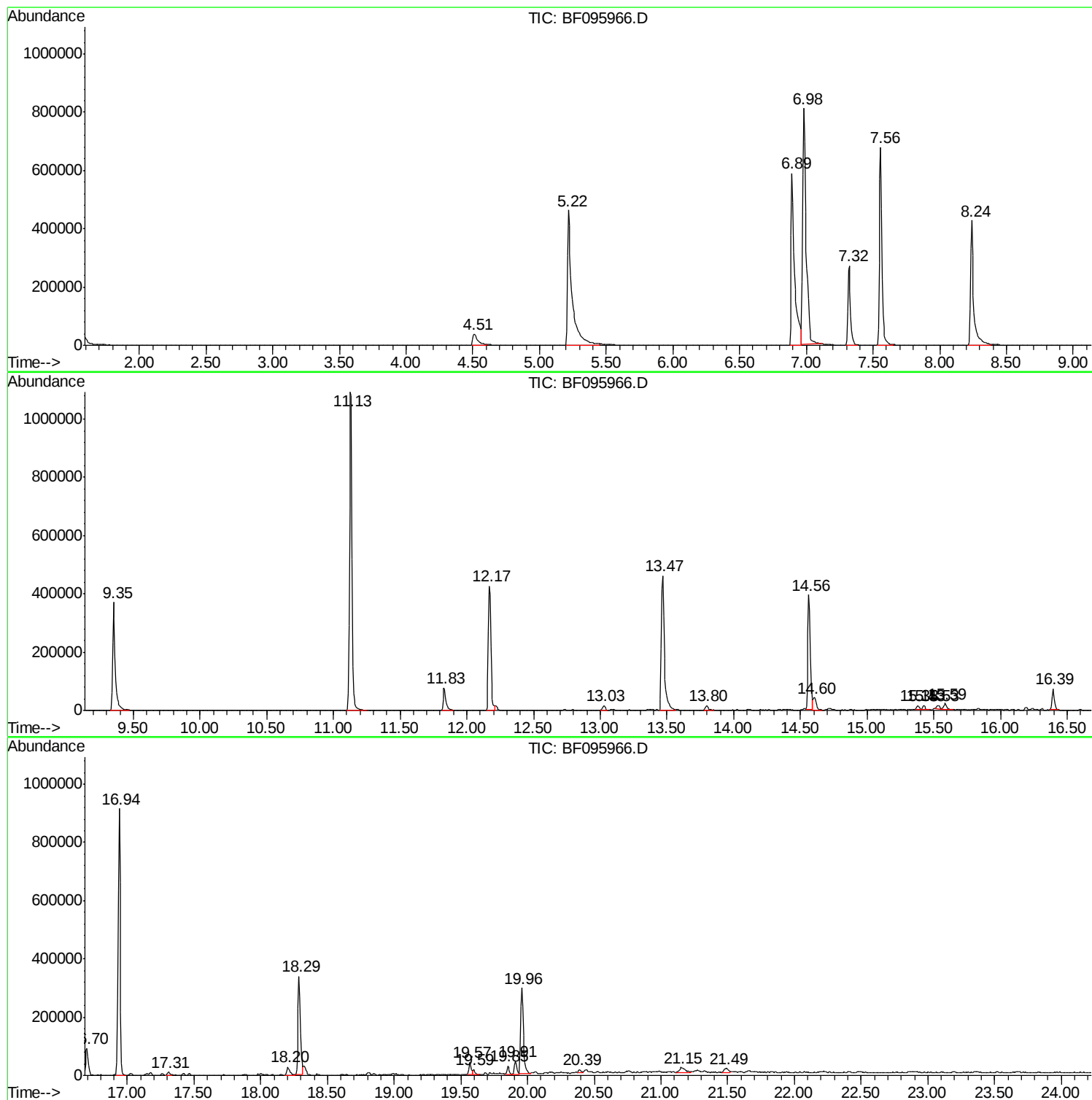
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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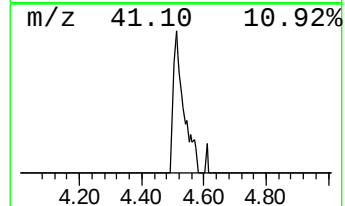
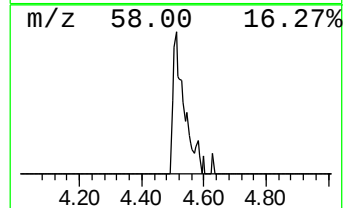
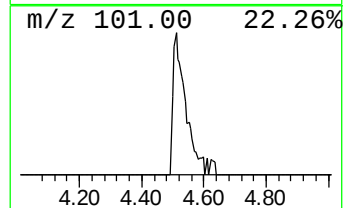
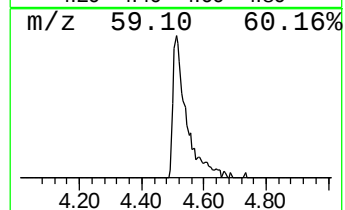
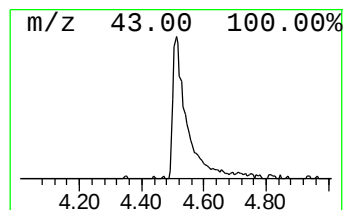
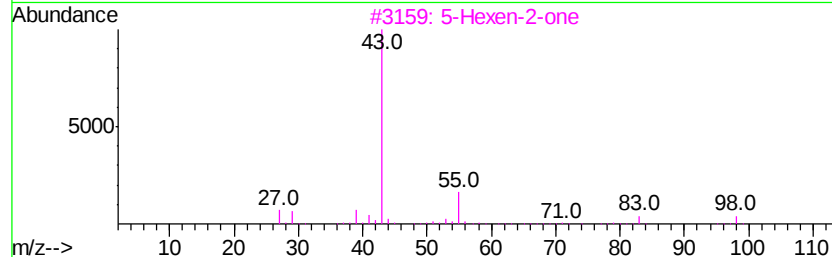
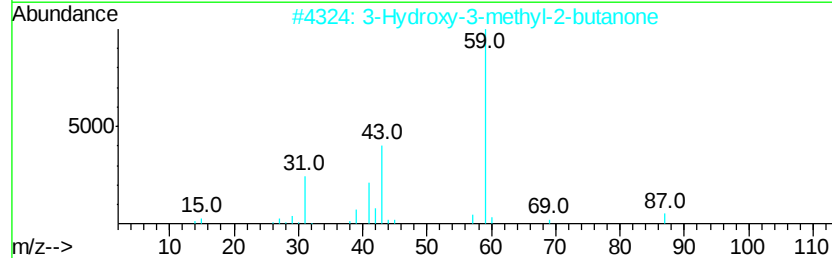
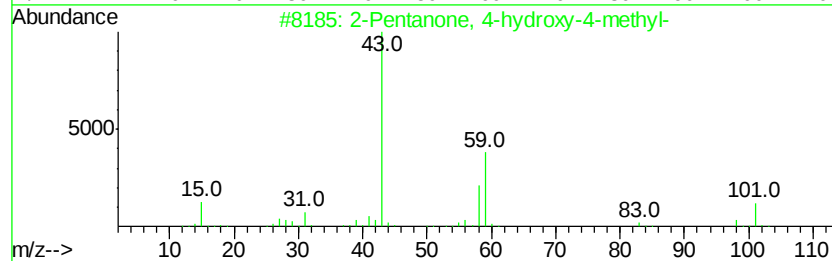
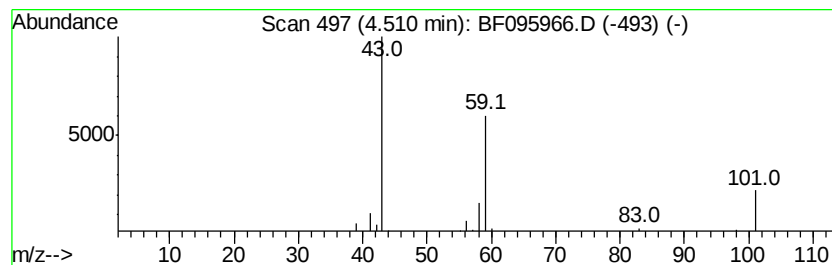
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.51	5.45 ng	102842	1,4-Dichlorobenzene-d4	7.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	



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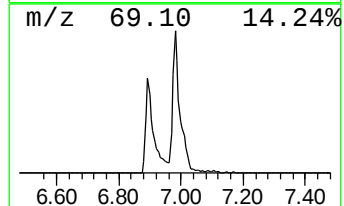
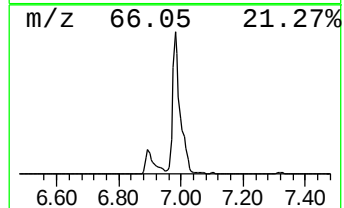
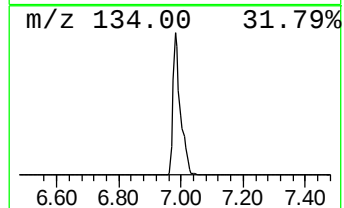
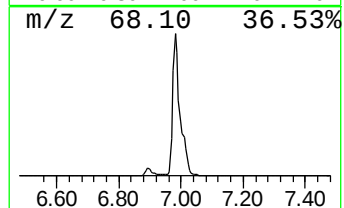
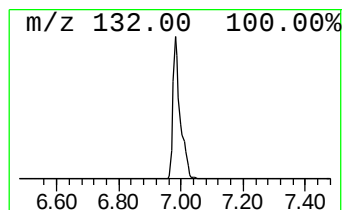
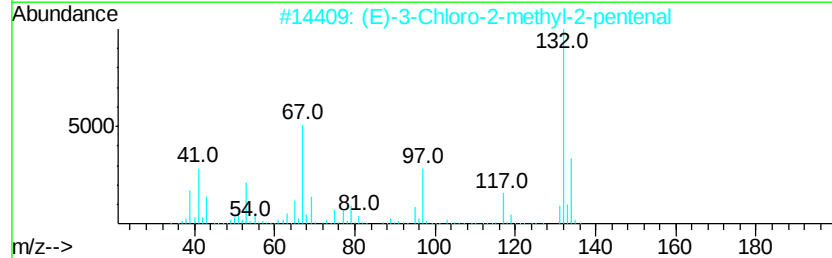
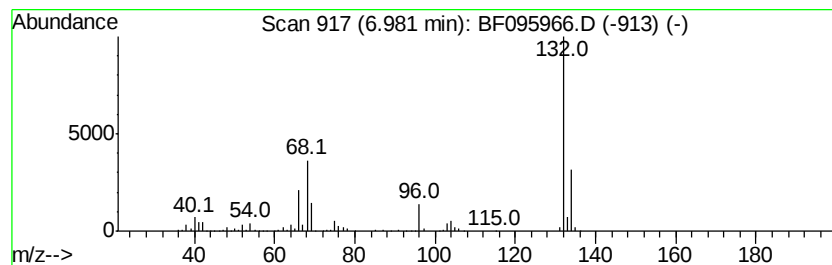
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	74.82 ng	1411290	1,4-Dichlorobenzene-d4	7.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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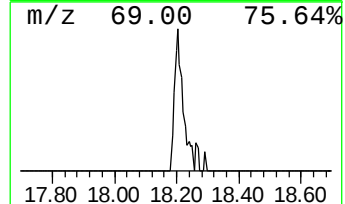
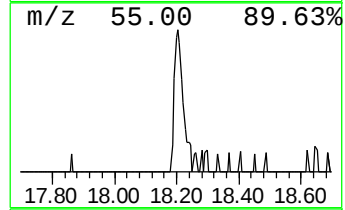
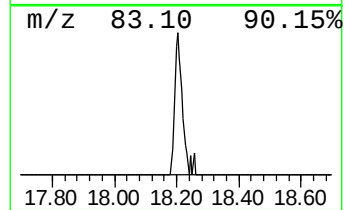
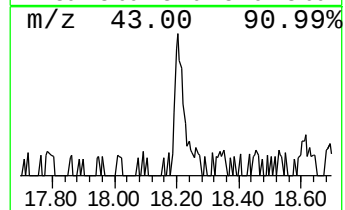
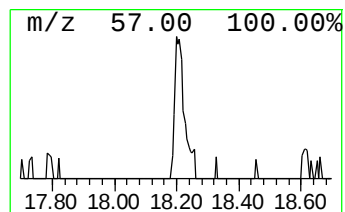
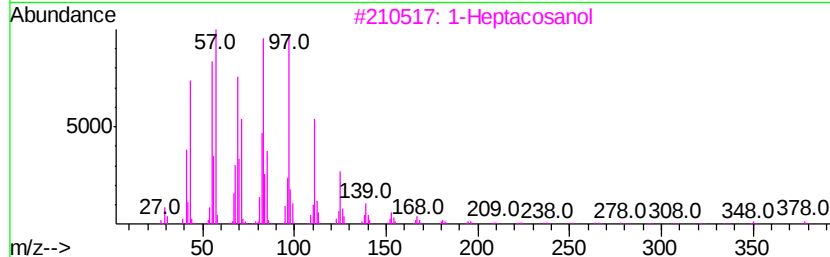
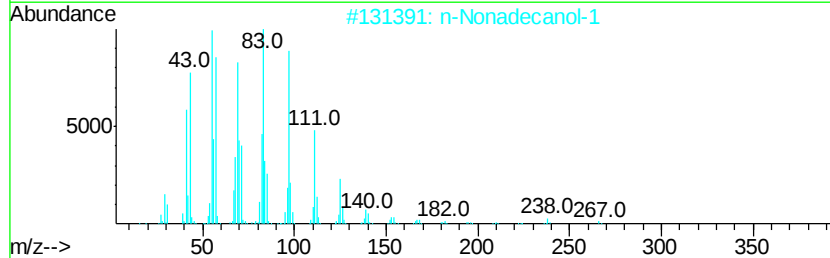
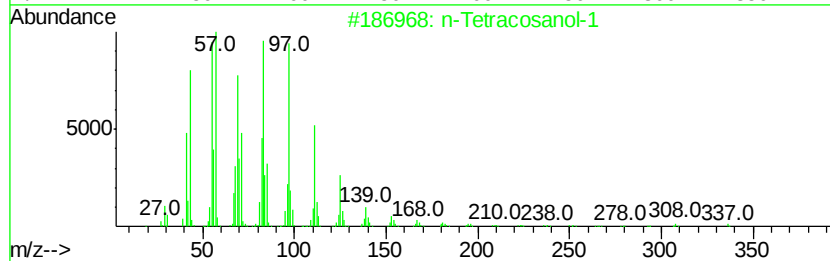
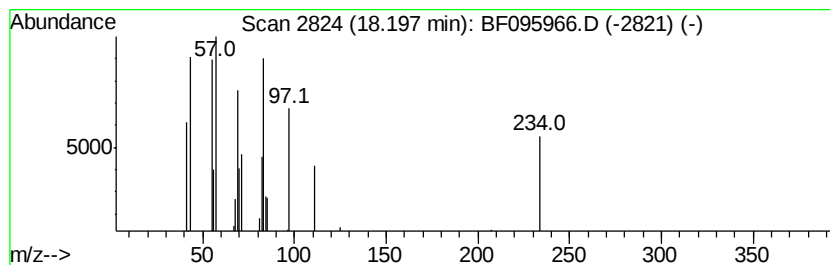
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.20	2.23 ng	47616	Chrysene-d12	18.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93	
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93	
3	1-Heptacosanol	396	C27H56O	002004-39-9	93	
4	1-Heneicosanol	312	C21H44O	015594-90-8	93	
5	Behenic alcohol	326	C22H46O	000661-19-8	93	



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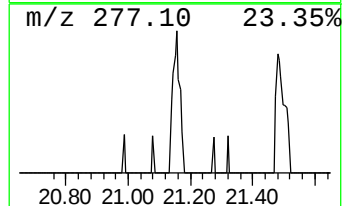
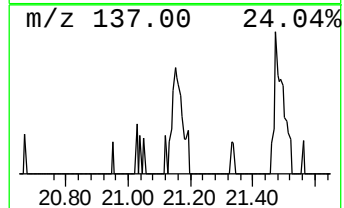
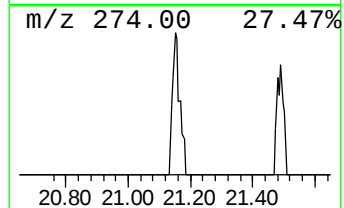
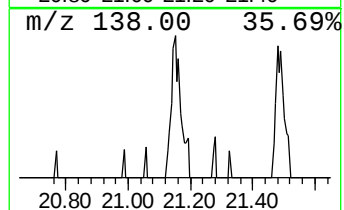
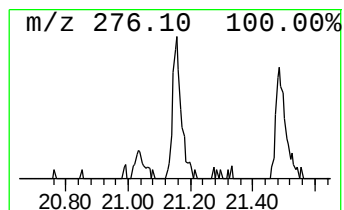
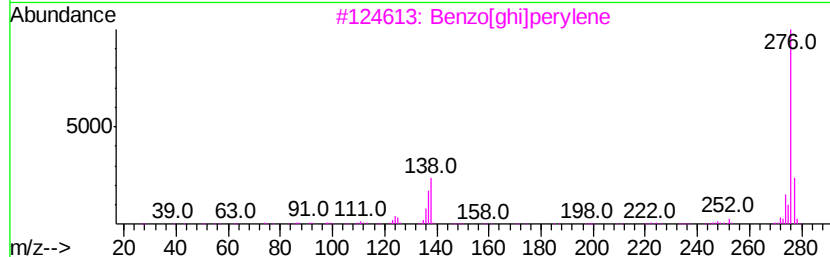
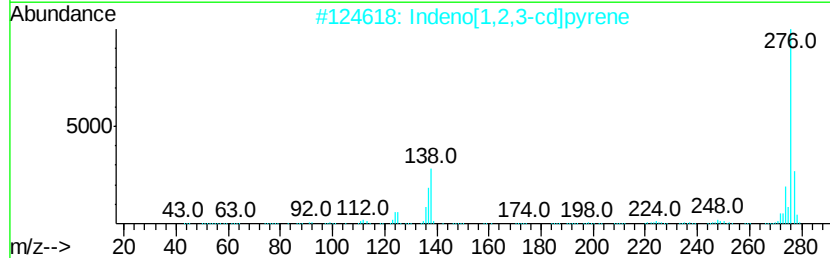
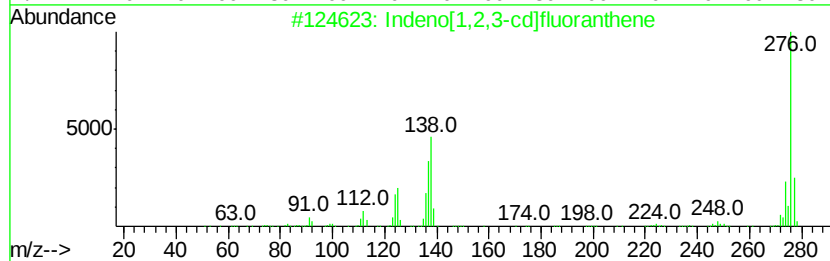
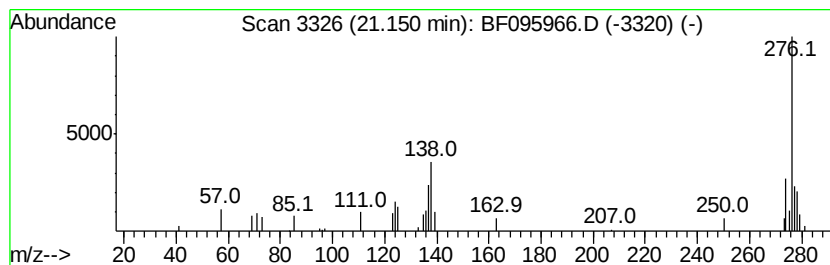
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indeno[1,2,3-cd]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	2.11 ng	42925	Perylene-d12	19.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	76
2		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	76
3		Benzo[ghi]perylene	276	C22H12	000191-24-2	70
4		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	68
5		2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.51	5.5	ng	102842	1	7.32	377260	20.0
unknown6.98	6.98	74.8	ng	1411290	1	7.32	377260	20.0
n-Tetracosanol-1	18.20	2.2	ng	47616	5	18.29	426688	20.0
Indeno[1,2,3-cd]f...	21.15	2.1	ng	42925	6	19.96	407103	20.0