

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
 Data File : BM029608.D
 Acq On : 22 Apr 2021 23:46
 Operator : CG/JU
 Sample : M2106-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-24-14.5-15.0

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_M\Methods\8270-BM042121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.228	392	398	419	rBV	947760	1406547	41.89%	6.772%
2	6.810	656	667	683	rBV	909725	1466814	43.69%	7.062%
3	7.633	800	807	814	rBV	238797	389734	11.61%	1.876%
4	8.786	996	1003	1025	rBV	517558	902410	26.88%	4.345%
5	10.410	1271	1279	1287	rBV	296211	501038	14.92%	2.412%
6	12.892	1694	1701	1714	rBV	1525695	2188280	65.18%	10.536%
7	13.739	1840	1845	1854	rVB	43289	62342	1.86%	0.300%
8	14.274	1929	1936	1944	rBV	472104	690911	20.58%	3.327%
9	15.768	2180	2190	2203	rBV	1154754	1679003	50.01%	8.084%
10	17.021	2396	2403	2415	rBV	530373	826940	24.63%	3.982%
11	17.927	2552	2557	2567	rBV2	122159	207937	6.19%	1.001%
12	18.862	2712	2716	2722	rVB	45248	57778	1.72%	0.278%
13	19.209	2771	2775	2782	rBV6	38689	73739	2.20%	0.355%
14	19.468	2815	2819	2831	rVB	318377	487238	14.51%	2.346%
15	19.650	2845	2850	2862	rVB	2837457	3357523	100.00%	16.166%
16	19.974	2902	2905	2909	rVB	90161	94921	2.83%	0.457%
17	20.468	2986	2989	2994	rVB	102957	114305	3.40%	0.550%
18	20.927	3063	3067	3076	rBV	430421	568662	16.94%	2.738%
19	21.197	3109	3113	3121	rBV	796039	1029919	30.67%	4.959%
20	21.368	3138	3142	3146	rBV	132139	155736	4.64%	0.750%
21	21.791	3211	3214	3225	rVB3	137140	217200	6.47%	1.046%
22	22.244	3288	3291	3295	rVB	82120	94503	2.81%	0.455%
23	22.468	3325	3329	3333	rBV	199167	260812	7.77%	1.256%
24	22.738	3372	3375	3379	rVB	109508	150624	4.49%	0.725%
25	23.391	3480	3486	3492	rVB2	598946	1106395	32.95%	5.327%
26	25.803	3888	3896	3908	rVB	982467	2678062	79.76%	12.894%

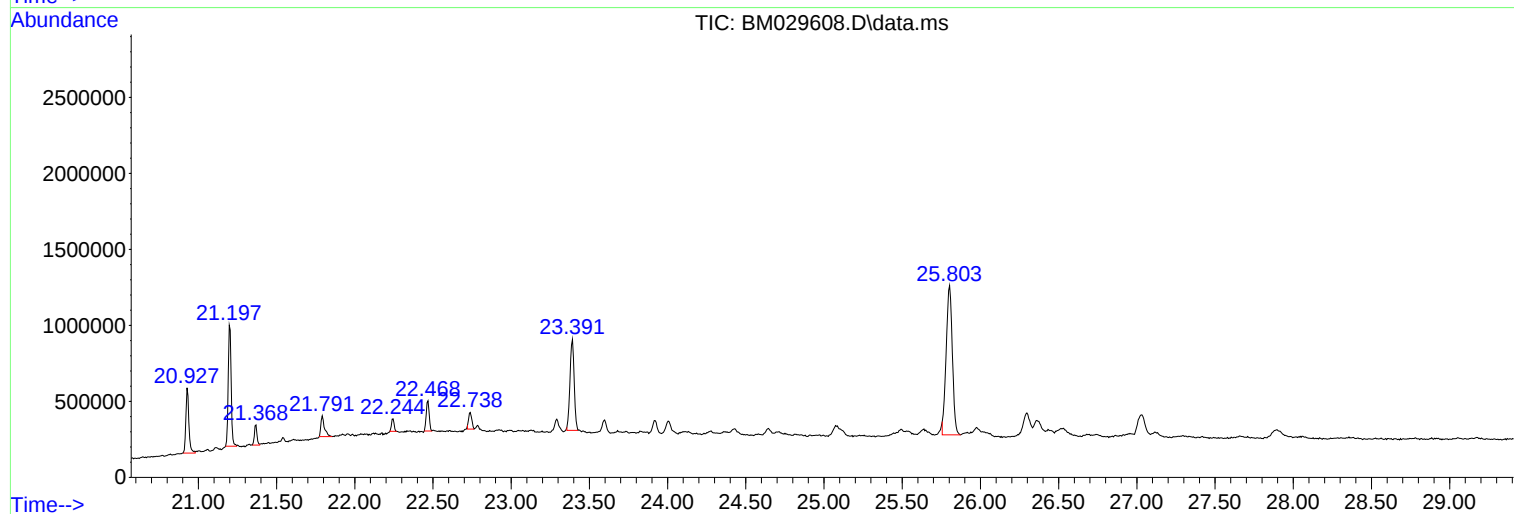
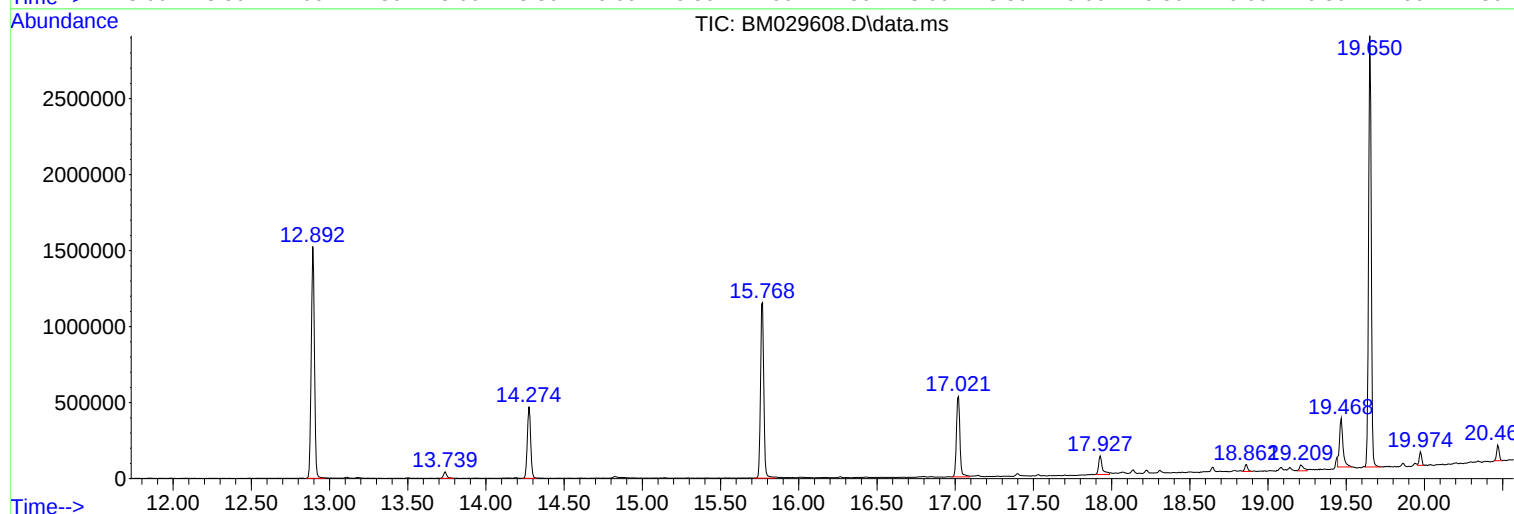
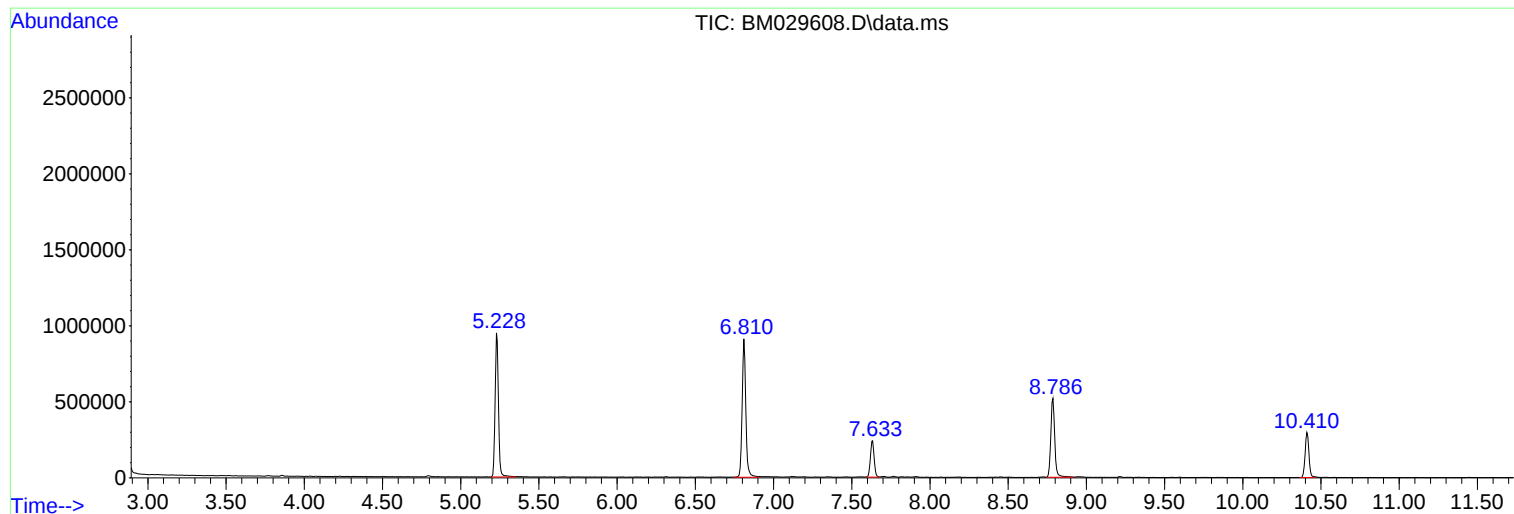
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Instrument :
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ClientSampleId :
SB-24-14.5-15.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.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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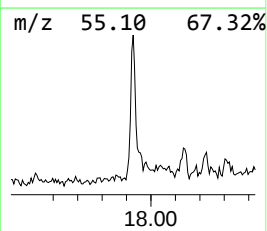
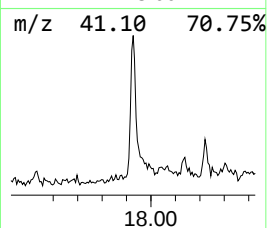
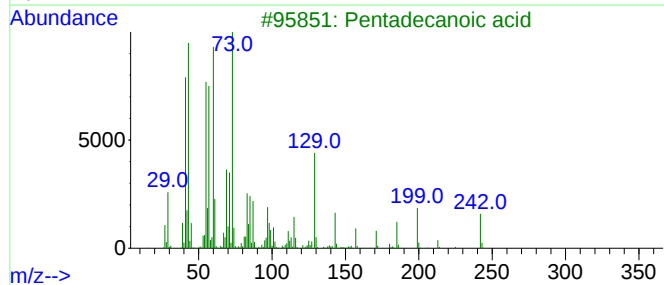
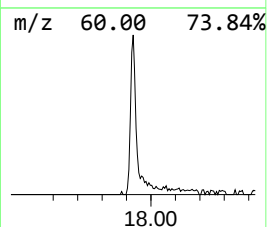
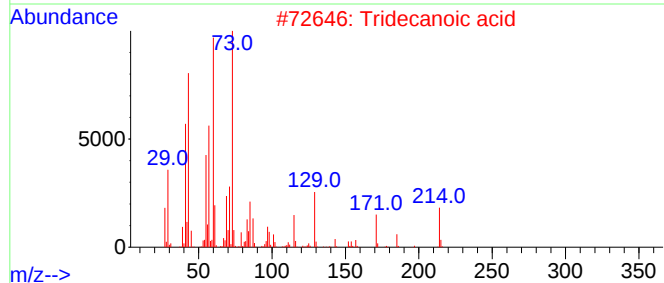
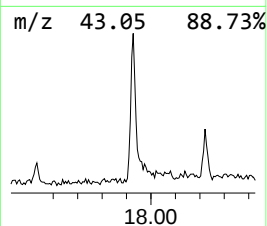
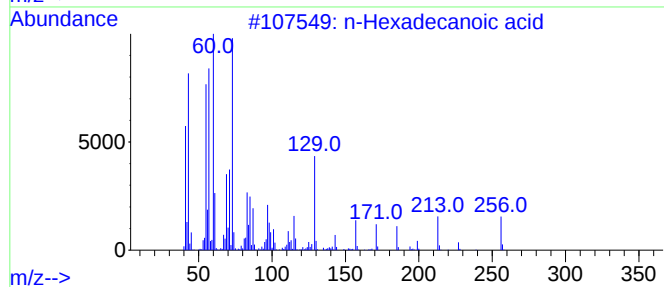
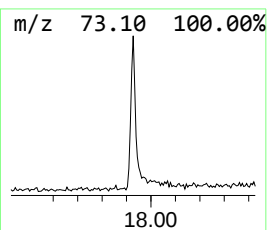
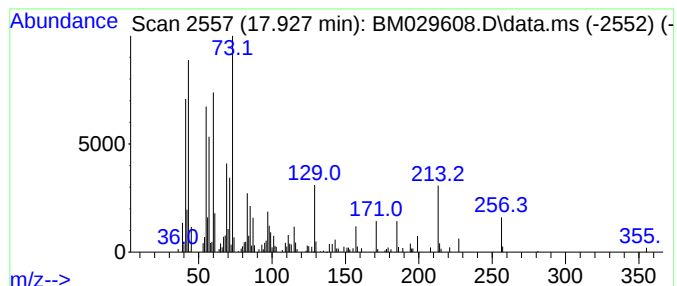
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.927	5.03 ng	207937	Phenanthrene-d10	17.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Octadecanoic acid	284	C18H36O2	000057-11-4	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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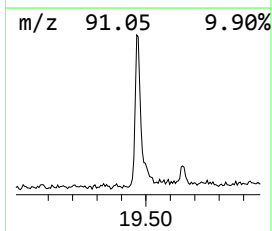
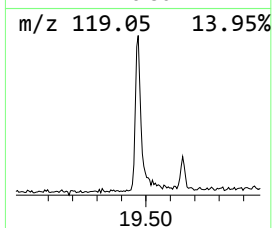
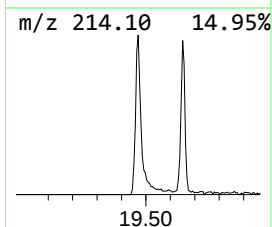
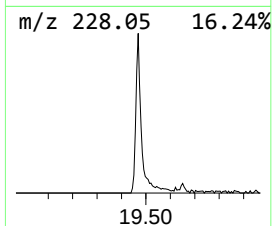
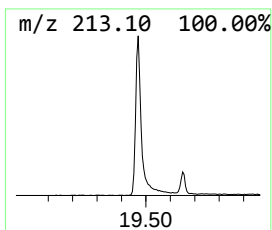
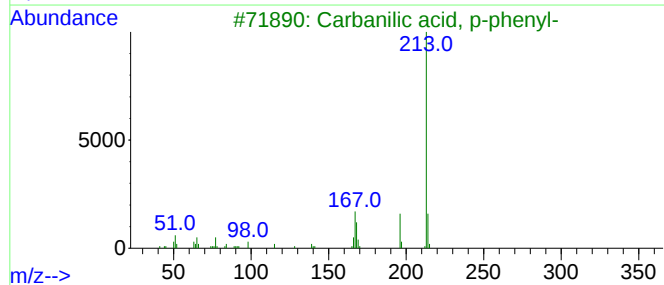
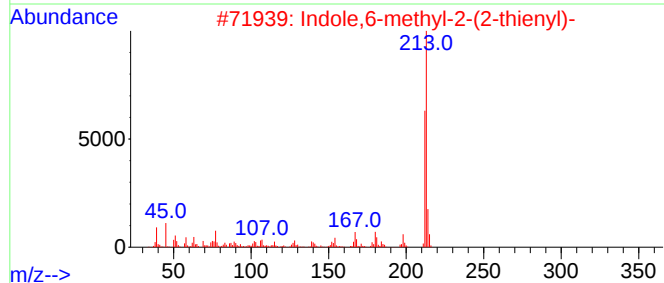
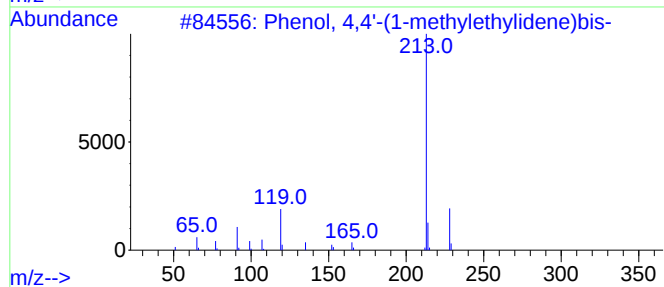
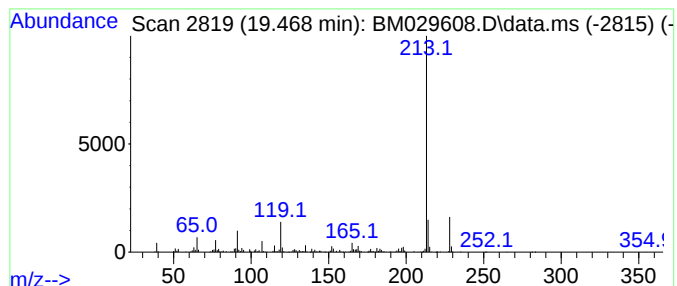
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Peak Number 2 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	9.46 ng	487238	Chrysene-d12	21.197

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	95
2			Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	50
3			Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50
4			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	45
5			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	42



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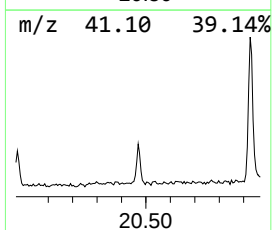
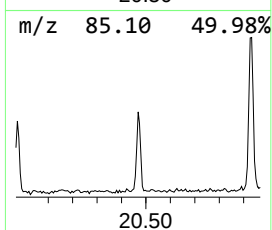
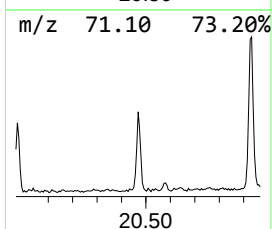
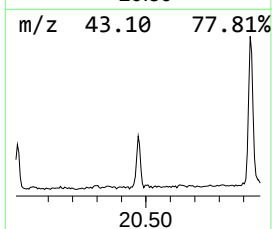
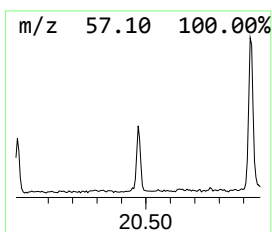
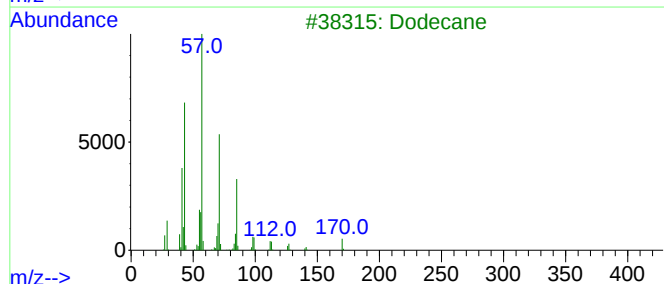
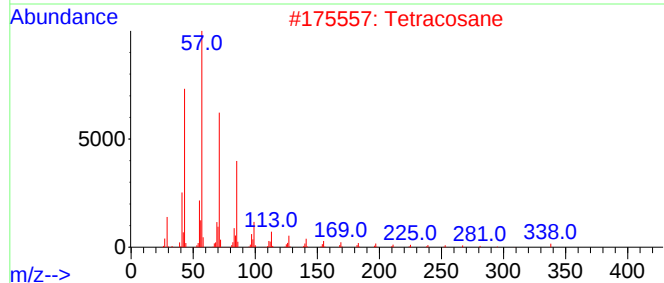
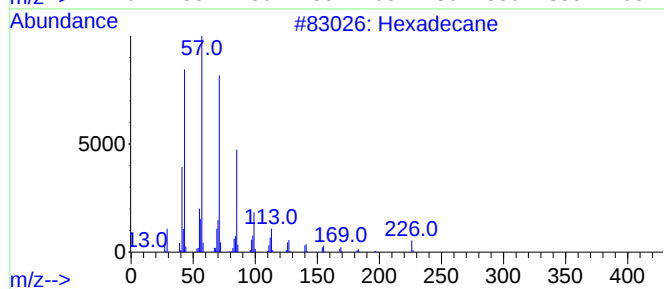
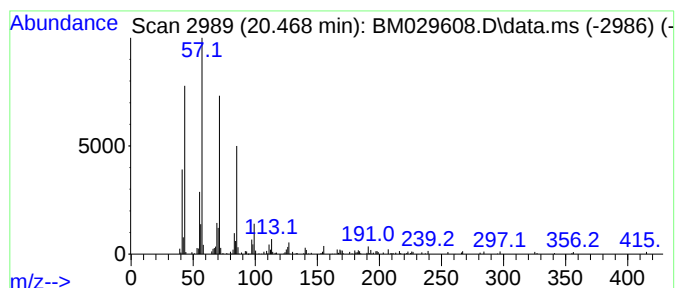
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.468	2.22 ng	114305	Chrysene-d12	21.197

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	89
2			Tetracosane	338	C24H50	000646-31-1	87
3			Dodecane	170	C12H26	000112-40-3	87
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86



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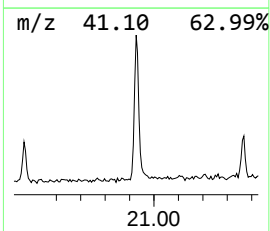
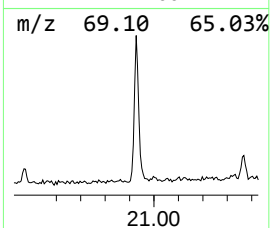
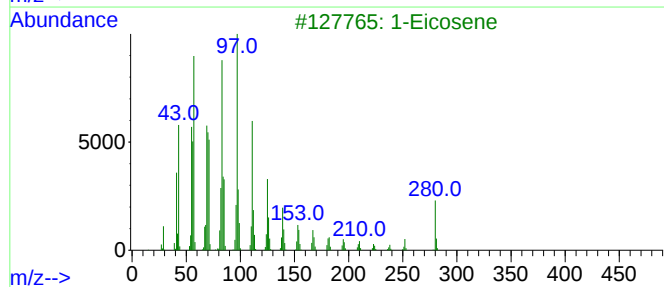
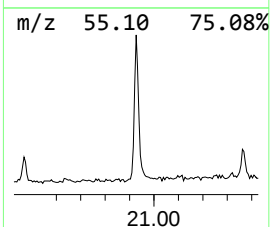
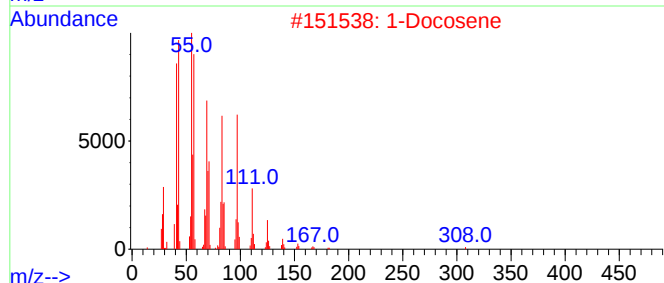
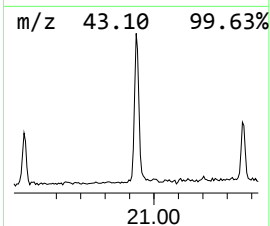
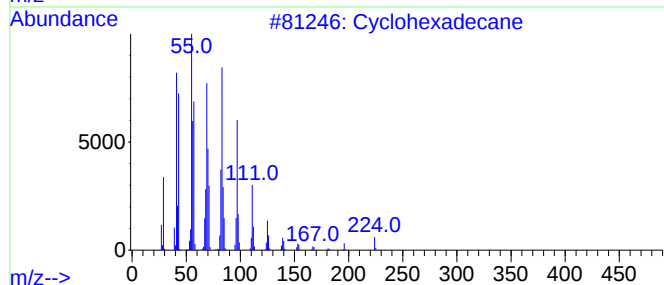
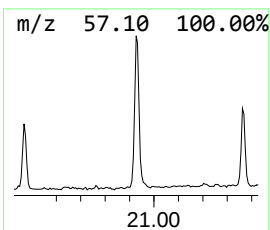
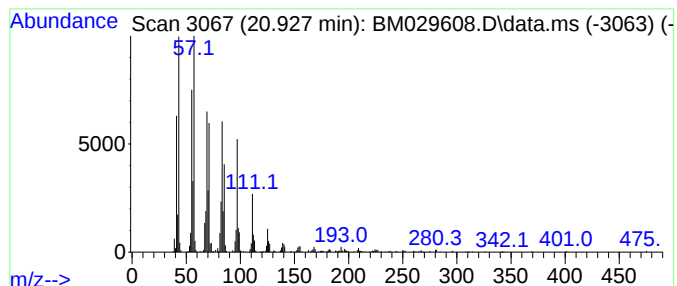
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Peak Number 4 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	11.04 ng	568662	Chrysene-d12	21.197

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			1-Docosene	308	C22H44	001599-67-3	93
3			1-Eicosene	280	C20H40	003452-07-1	93
4			Cyclotetradecane	196	C14H28	000295-17-0	92
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



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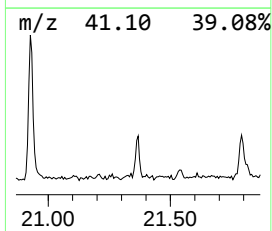
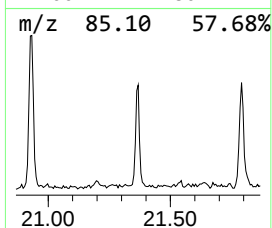
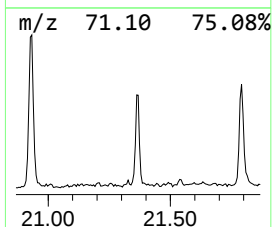
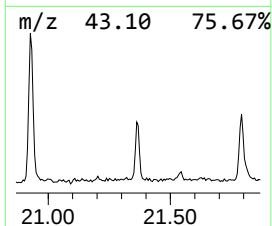
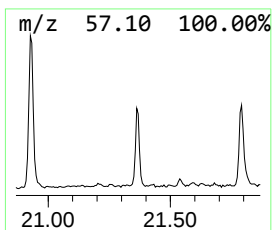
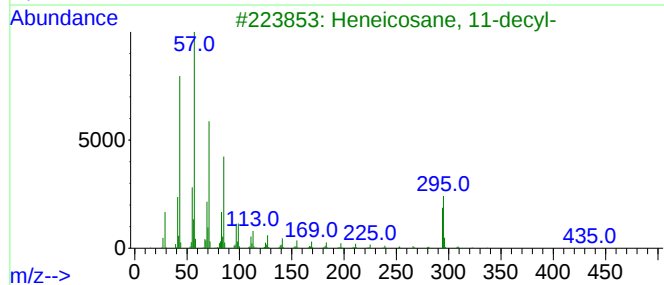
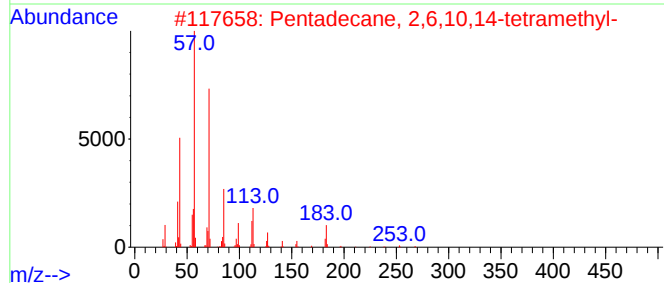
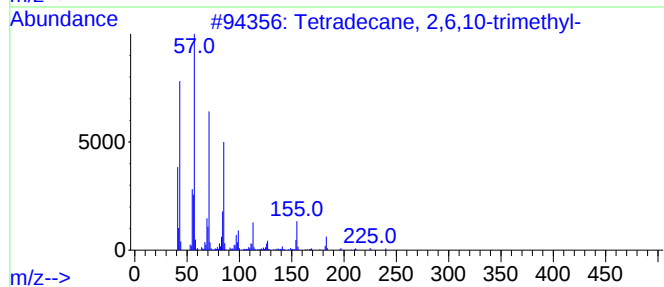
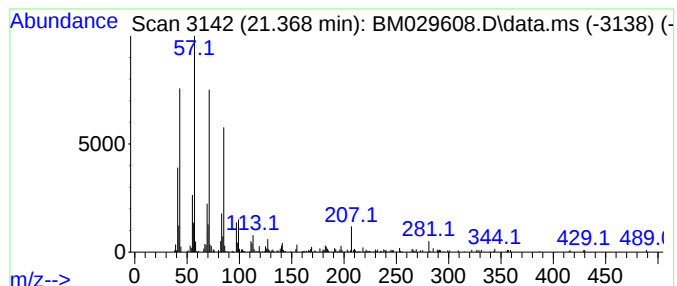
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Peak Number 5 Tetradecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.368	3.02 ng	155736	Chrysene-d12	21.197	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Tetracosane	338	C24H50	000646-31-1	83



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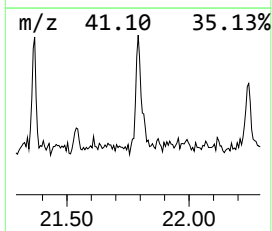
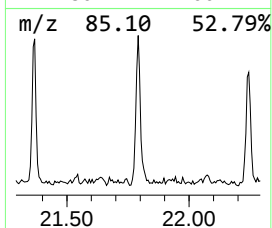
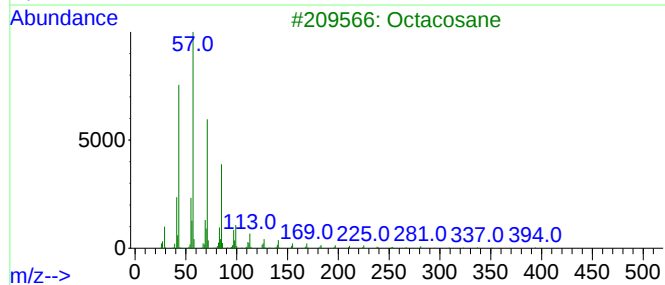
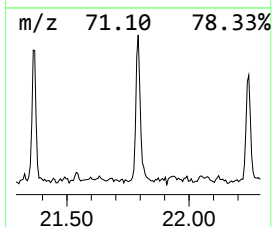
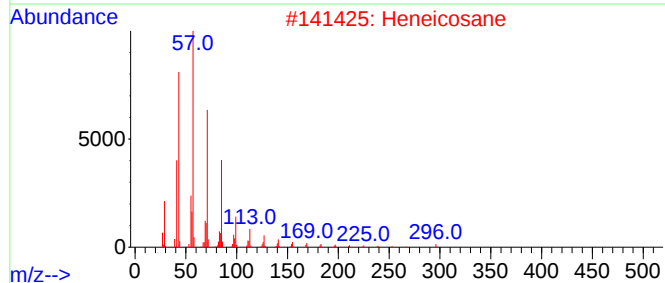
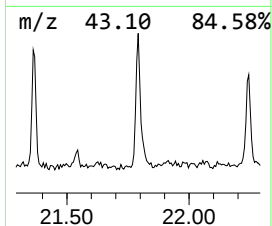
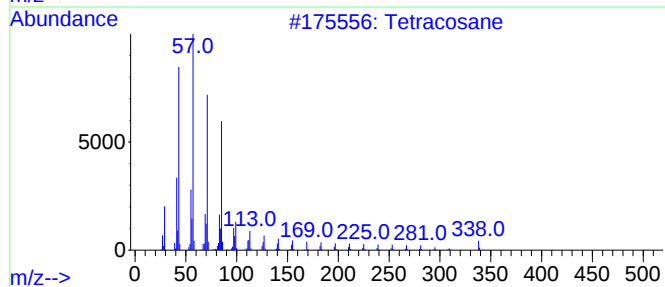
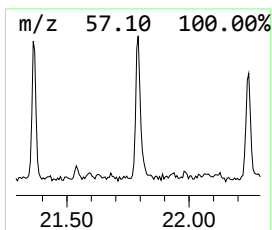
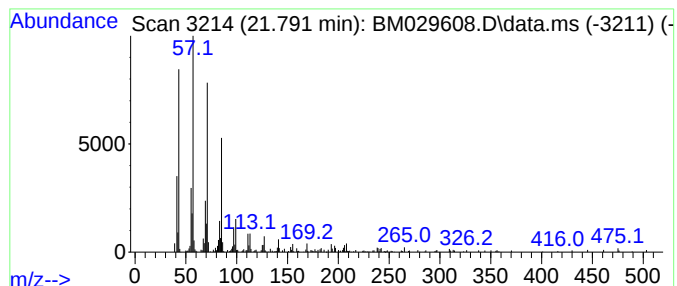
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.791	4.22 ng	217200	Chrysene-d12	21.197

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
Data File : BM029608.D
Acq On : 22 Apr 2021 23:46
Operator : CG/JU
Sample : M2106-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-24-14.5-15.0

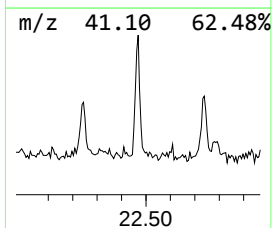
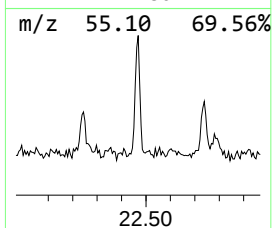
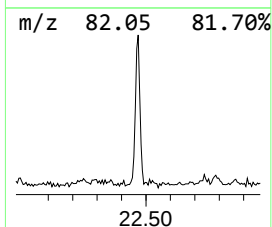
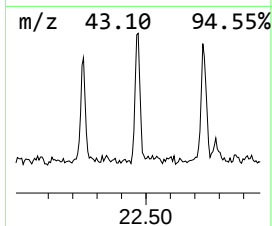
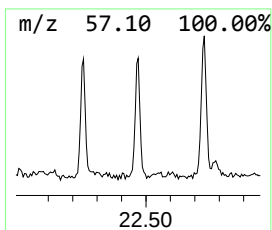
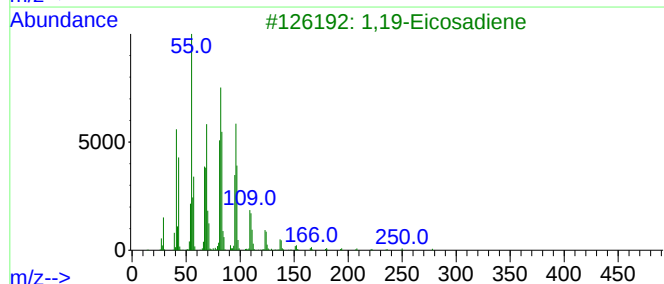
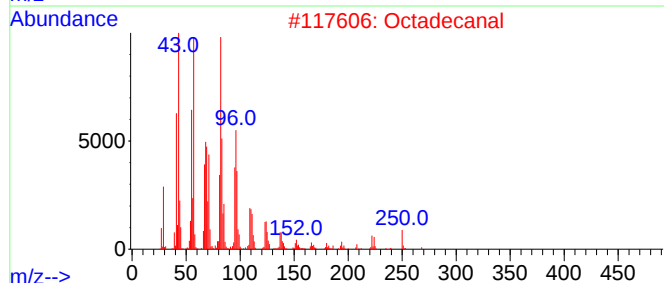
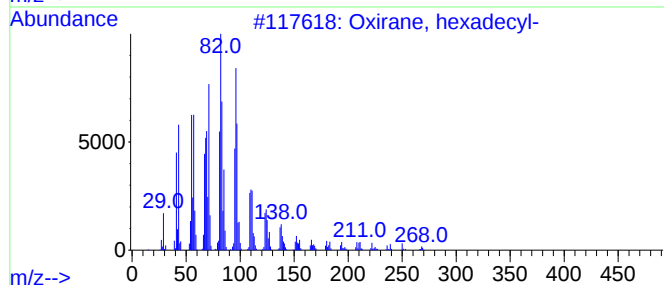
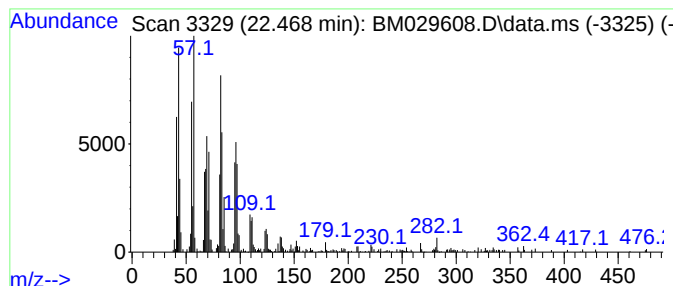
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.468	4.71 ng	260812	Perylene-d12	23.391

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	96
2			Octadecanal	268	C18H36O	000638-66-4	96
3			1,19-Eicosadiene	278	C20H38	014811-95-1	95
4			Pentadecanal-	226	C15H30O	002765-11-9	93
5			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
Data File : BM029608.D
Acq On : 22 Apr 2021 23:46
Operator : CG/JU
Sample : M2106-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-24-14.5-15.0

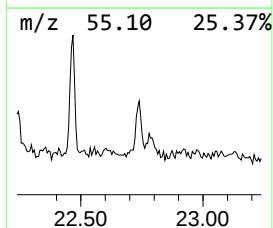
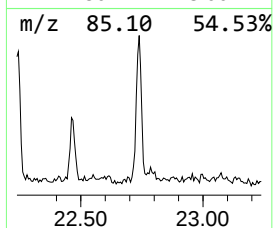
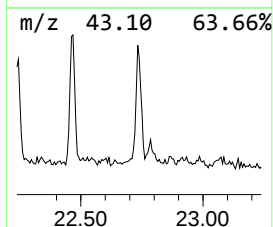
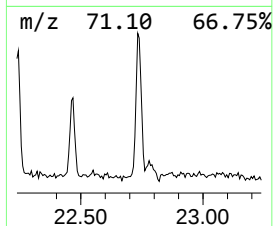
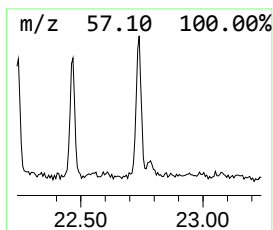
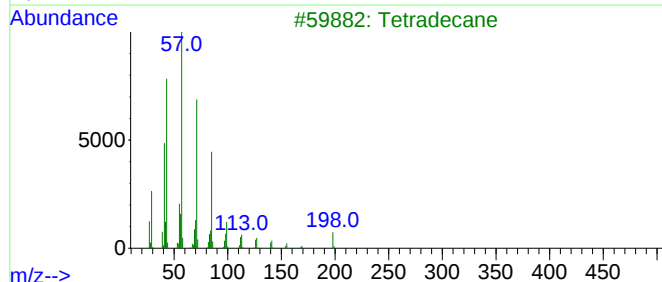
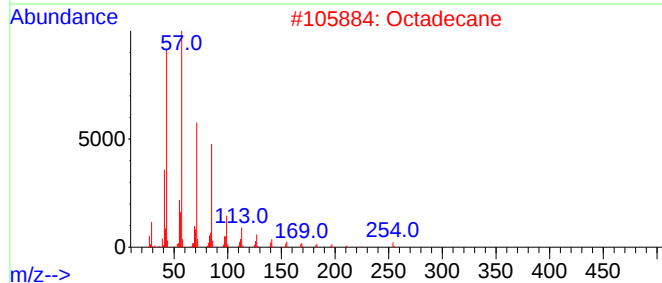
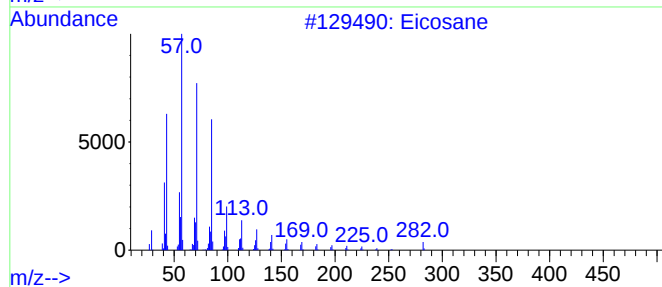
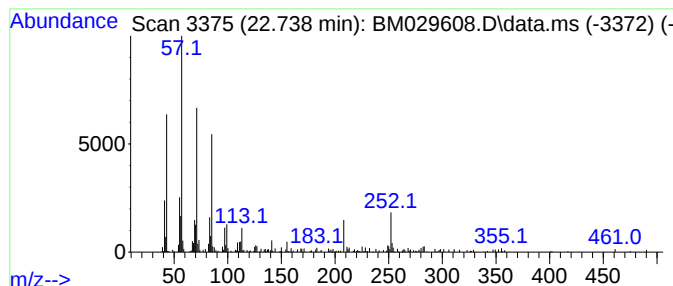
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.738	2.72 ng	150624	Perylene-d12	23.391

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	93
2	Octadecane			254	C18H38	000593-45-3	89
3	Tetradecane			198	C14H30	000629-59-4	89
4	Nonadecane			268	C19H40	000629-92-5	89
5	Pentacosane			352	C25H52	000629-99-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
Data File : BM029608.D
Acq On : 22 Apr 2021 23:46
Operator : CG/JU
Sample : M2106-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-24-14.5-15.0

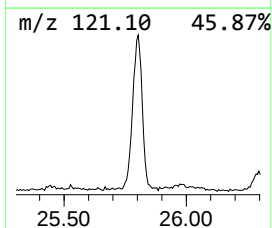
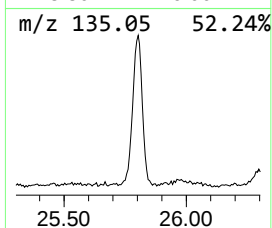
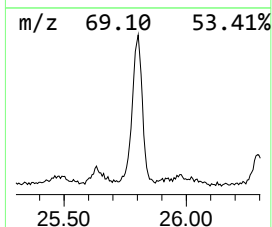
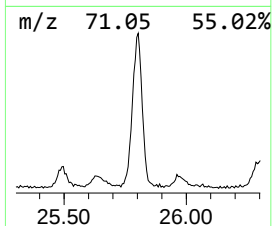
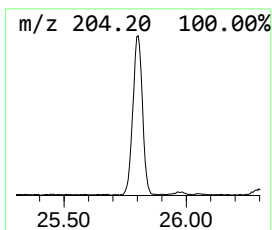
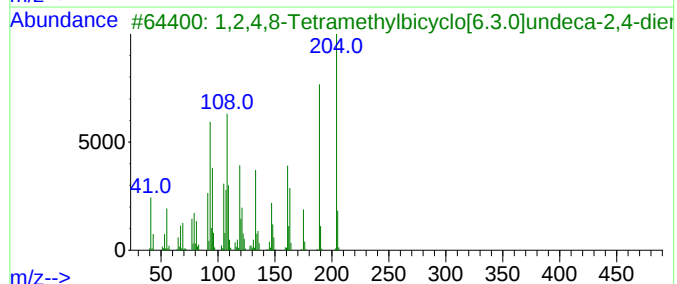
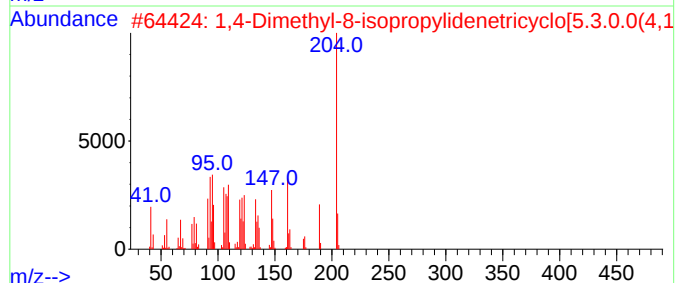
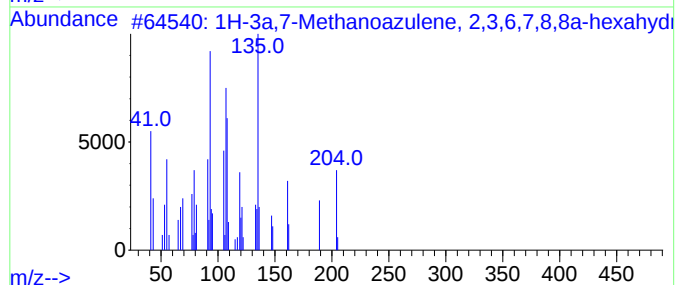
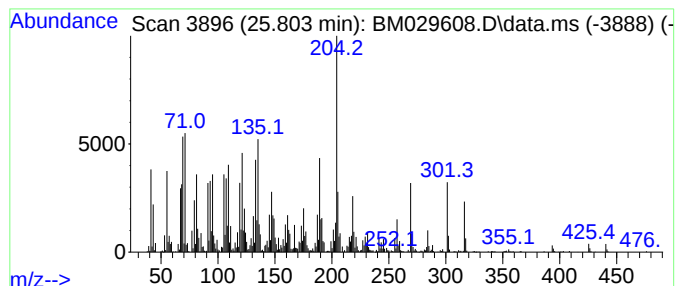
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown25.803 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.803	48.41 ng	2678060	Perylene-d12	23.391

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49
2			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	49
3			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	45
4			5-(2,4-Dichloro-phenoxymethyl)-4...	365	C16H13Cl2N3OS	1000296-81-4	45
5			2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
Data File : BM029608.D
Acq On : 22 Apr 2021 23:46
Operator : CG/JU
Sample : M2106-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-24-14.5-15.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.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
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Phenol, 4,4'-(1...	19.468	9.5	ng	487238	5	21.197	1029920	20.0
Hexadecane	20.468	2.2	ng	114305	5	21.197	1029920	20.0
Cyclohexadecane	20.927	11.0	ng	568662	5	21.197	1029920	20.0
Tetradecane, 2,...	21.368	3.0	ng	155736	5	21.197	1029920	20.0
Tetracosane	21.791	4.2	ng	217200	5	21.197	1029920	20.0
Oxirane, hexade...	22.468	4.7	ng	260812	6	23.391	1106400	20.0
Eicosane	22.738	2.7	ng	150624	6	23.391	1106400	20.0
unknown25.803	25.803	48.4	ng	2678060	6	23.391	1106400	20.0