

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
 Data File : BP005271.D
 Acq On : 12 Apr 2021 17:59
 Operator : CG/JU
 Sample : M1967-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB2-A

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_P\Methods\8270E-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.817	290	294	303	rVB	312183	439085	23.88%	4.354%
2	5.275	368	372	379	rVB	499258	711316	38.68%	7.053%
3	6.864	636	642	656	rVB	643919	1032446	56.14%	10.237%
4	7.675	774	780	788	rVB	147666	227840	12.39%	2.259%
5	8.840	971	978	992	rBV	395517	651145	35.41%	6.456%
6	10.469	1248	1255	1260	rBV	157390	266157	14.47%	2.639%
7	11.981	1506	1512	1520	rBV	34222	59714	3.25%	0.592%
8	12.951	1669	1677	1692	rVB	828263	1167872	63.51%	11.580%
9	13.798	1816	1821	1828	rVB	24749	41775	2.27%	0.414%
10	14.057	1860	1865	1871	rBV	16078	25888	1.41%	0.257%
11	14.340	1906	1913	1919	rBV	244827	345045	18.76%	3.421%
12	15.840	2160	2168	2176	rBV	133707	198595	10.80%	1.969%
13	16.087	2204	2210	2215	rBV6	10468	20277	1.10%	0.201%
14	17.098	2376	2382	2387	rBV	299890	446434	24.28%	4.427%
15	17.145	2387	2390	2395	rVV	44989	62730	3.41%	0.622%
16	17.198	2395	2399	2402	rVV2	53749	68878	3.75%	0.683%
17	17.234	2402	2405	2411	rVB	28002	41190	2.24%	0.408%
18	18.163	2559	2563	2567	rBV2	21230	37163	2.02%	0.368%
19	18.869	2679	2683	2692	rBV7	14704	31191	1.70%	0.309%
20	18.998	2701	2705	2713	rBV7	17914	37542	2.04%	0.372%
21	19.122	2722	2726	2731	rBV	107876	141298	7.68%	1.401%
22	19.181	2733	2736	2741	rVB4	25781	35588	1.94%	0.353%
23	19.269	2749	2751	2756	rVB	17717	20064	1.09%	0.199%
24	19.480	2783	2787	2797	rVB2	108739	184103	10.01%	1.825%
25	19.680	2816	2821	2826	rVB	1621682	1838976	100.00%	18.234%
26	20.922	3028	3032	3039	rVB3	135881	271113	14.74%	2.688%
27	20.986	3039	3043	3051	rVB	209186	256935	13.97%	2.548%
28	21.116	3062	3065	3068	rVB	59195	65063	3.54%	0.645%
29	21.204	3074	3080	3084	rBV2	469230	671173	36.50%	6.655%
30	21.239	3084	3086	3092	rVB	85626	103209	5.61%	1.023%
31	22.780	3344	3348	3354	rBV3	62880	142242	7.73%	1.410%
32	23.474	3461	3466	3473	rVB2	245642	443107	24.10%	4.394%

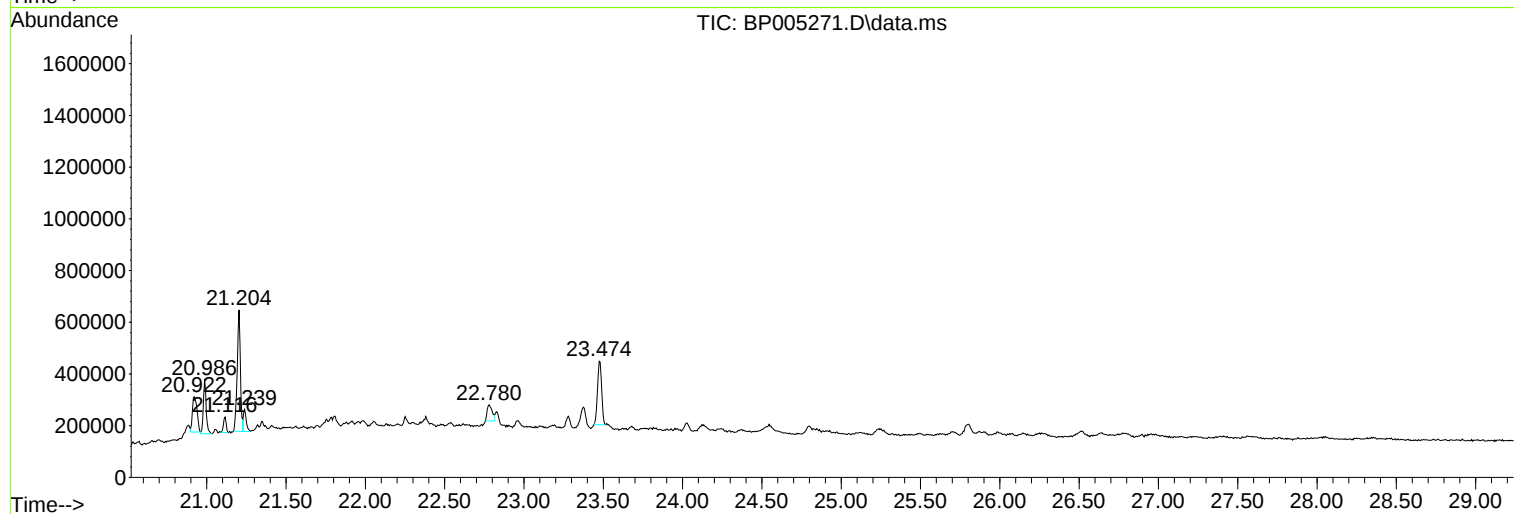
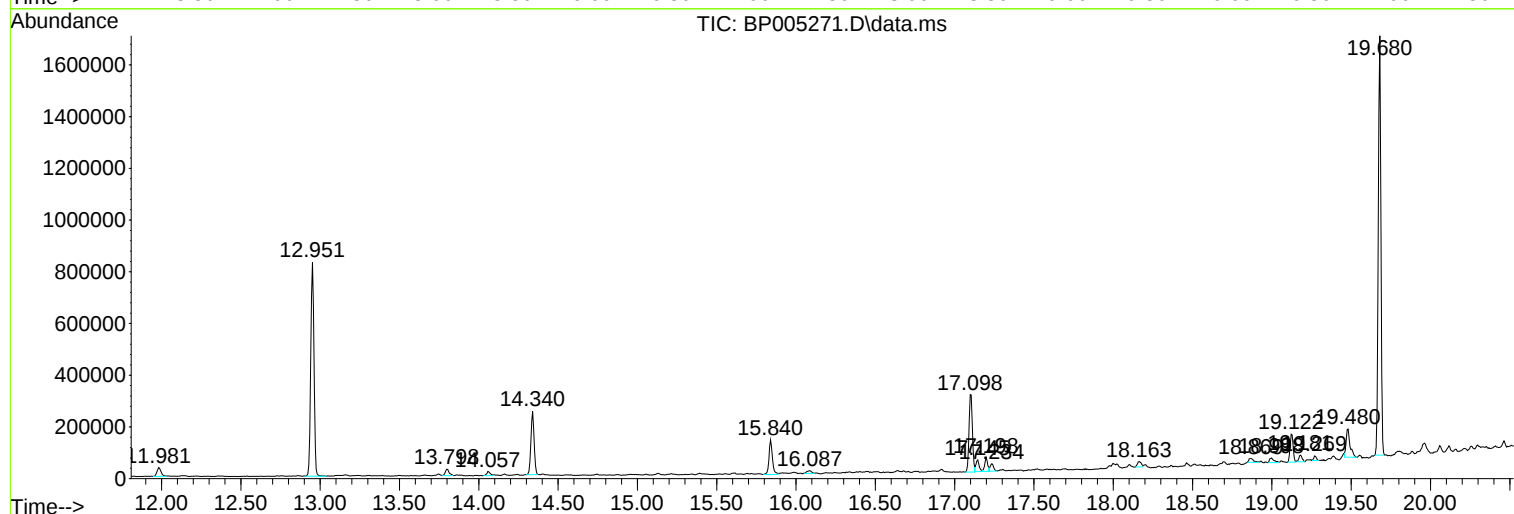
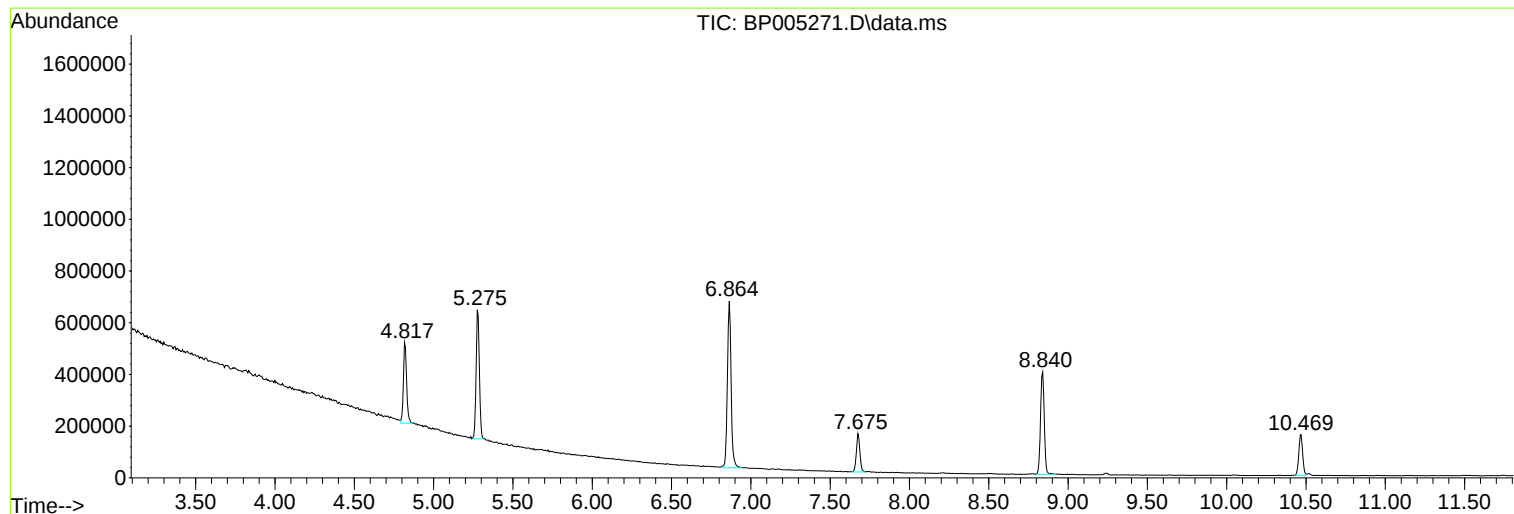
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ClientSampleId :
SB2-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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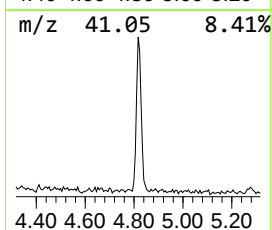
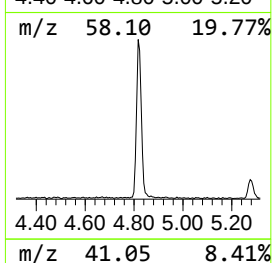
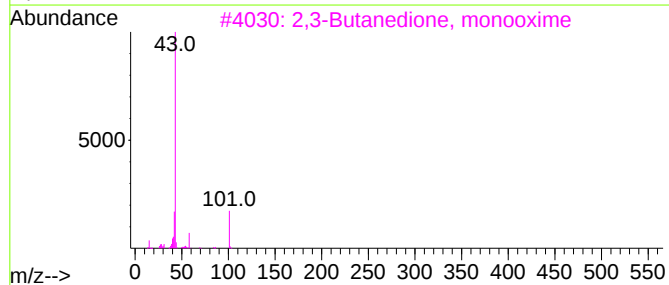
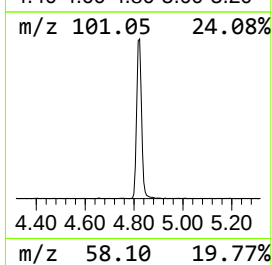
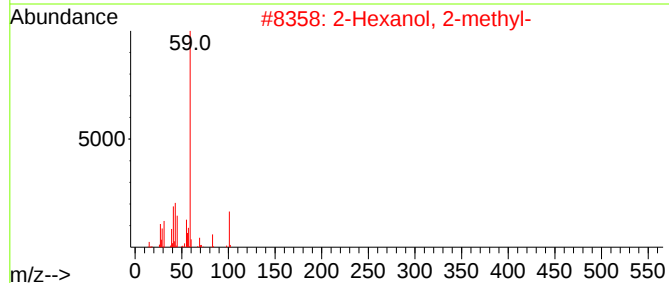
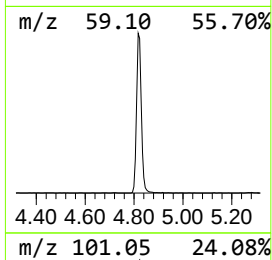
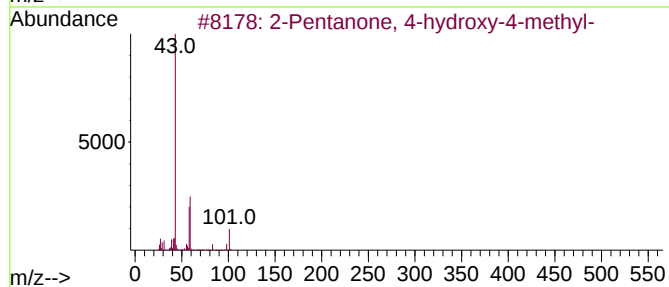
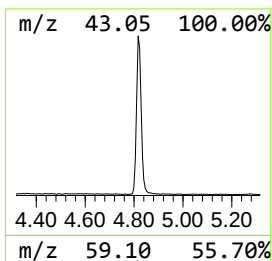
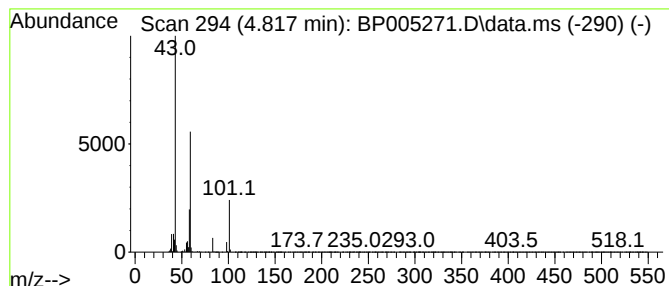
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.817	38.54 ng	439085	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	12		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12		



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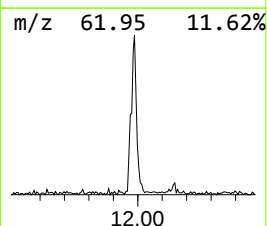
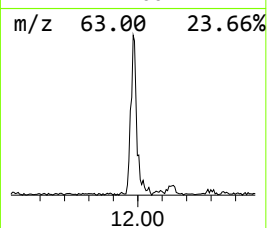
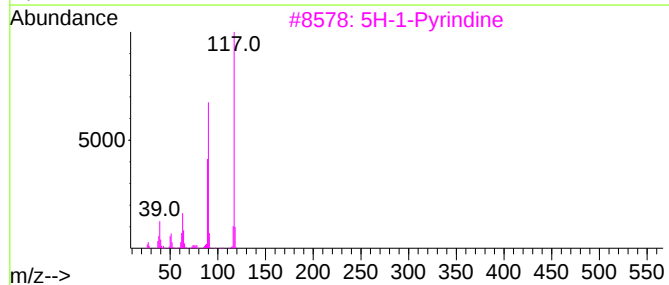
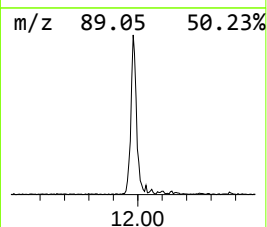
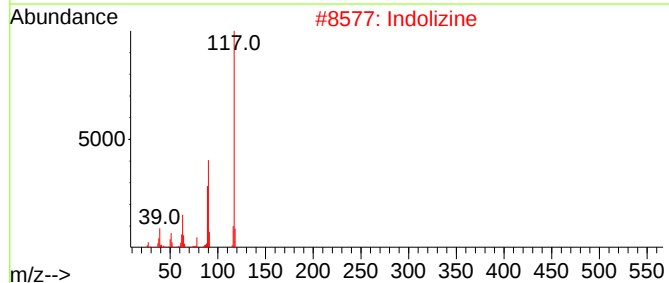
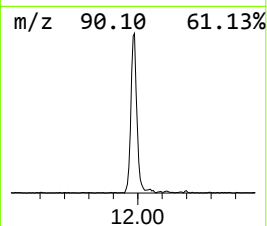
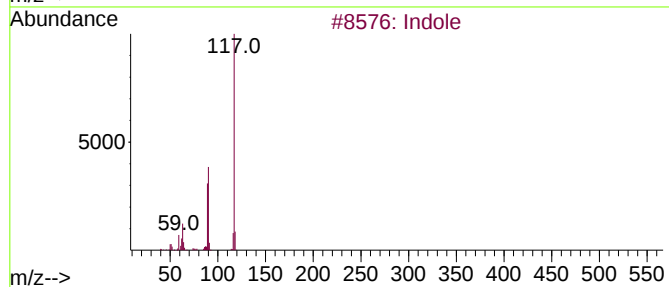
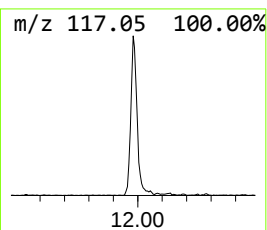
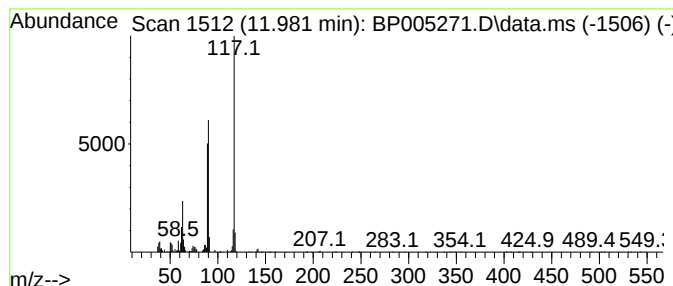
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Indole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	4.49 ng	59714	Naphthalene-d8	10.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			Indolizine	117	C8H7N	000274-40-8	91
3			5H-1-Pyridine	117	C8H7N	000270-91-7	90
4			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	87
5			Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	86



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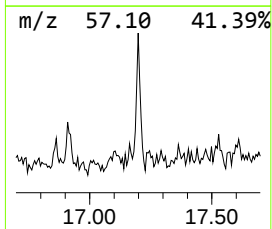
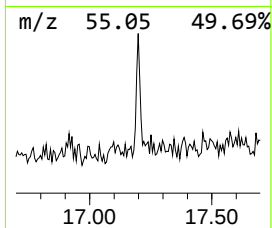
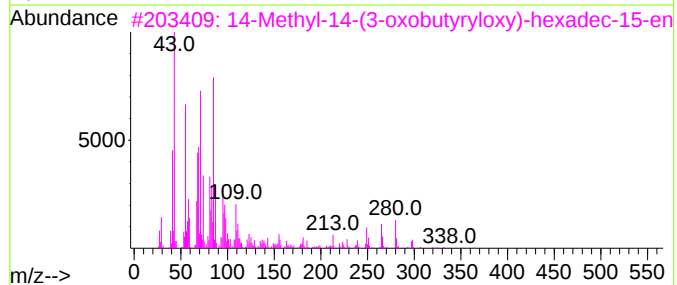
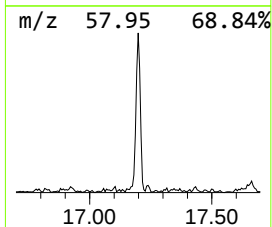
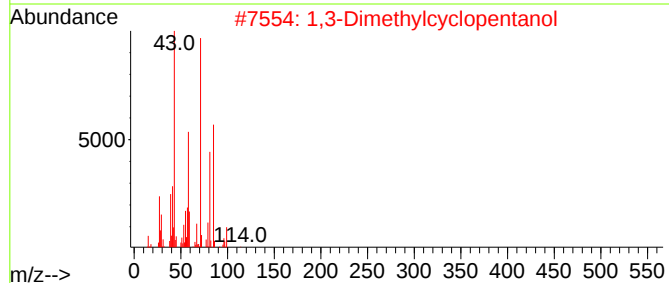
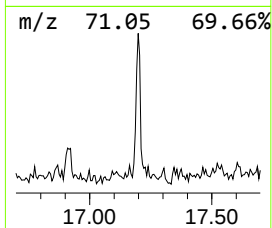
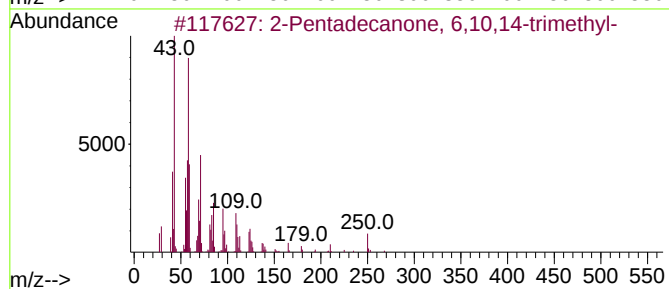
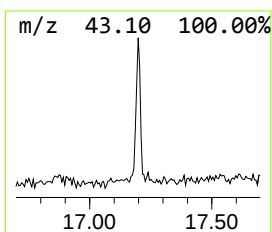
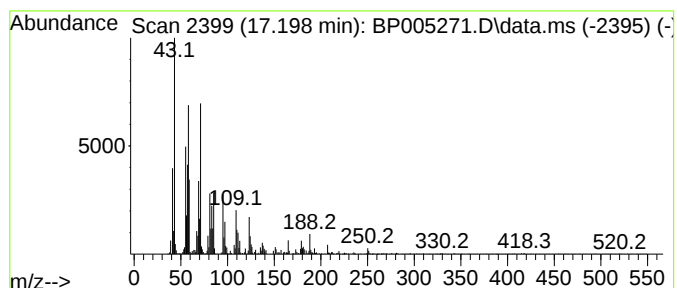
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentadecanone, 6,10,14-tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.198	3.09 ng	68878	Phenanthrene-d10	17.098	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	64
2	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	38
3	14-Methyl-14-(3-oxobutyryloxy)-h...	382	C22H38O5	1000192-92-9	38
4	Phytol	296	C20H40O	000150-86-7	27
5	2,2,5-Trimethyl-4,5-tetramethyle...	182	C10H18N2O	064934-87-8	25



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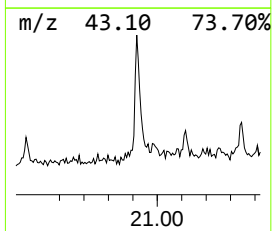
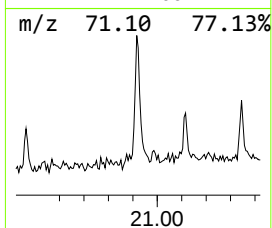
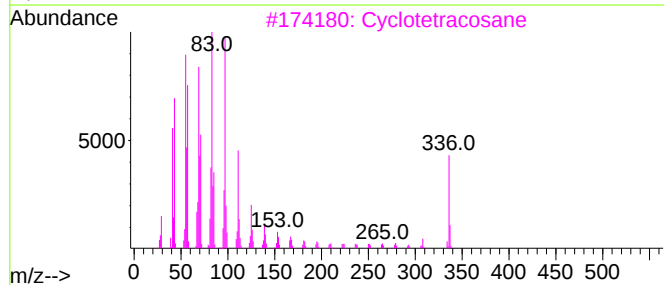
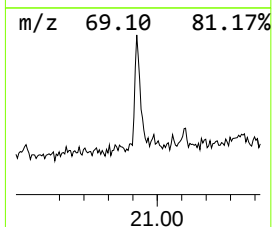
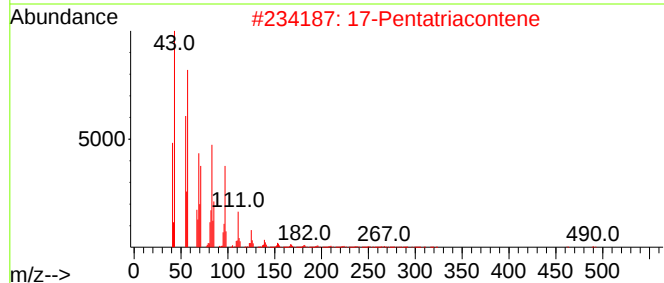
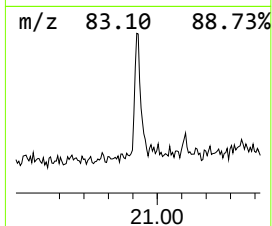
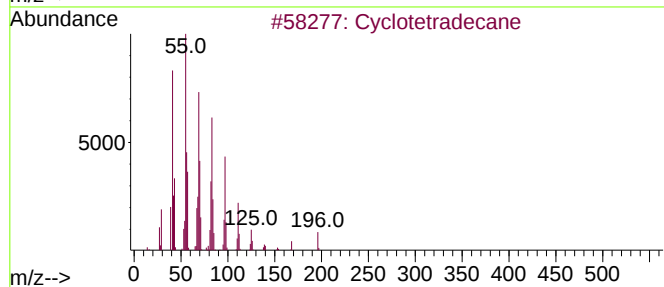
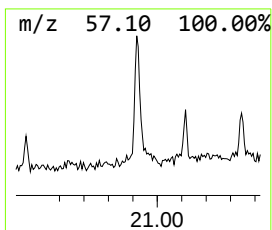
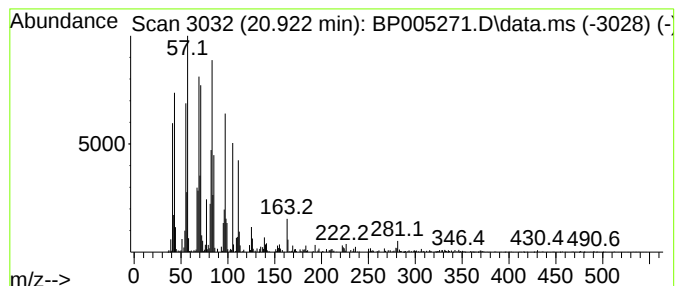
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Peak Number 4 Cyclotetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	8.08 ng	271113	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	90
3			Cyclotetracosane	336	C24H48	000297-03-0	89
4			1-Triacontanol	438	C30H62O	000593-50-0	83
5			Octadecane, 1-(ethenyl)-	296	C20H40O	000930-02-9	76



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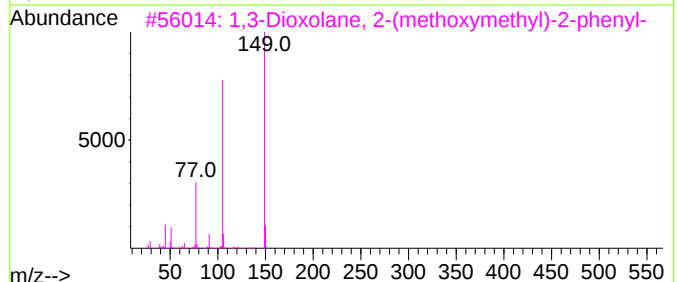
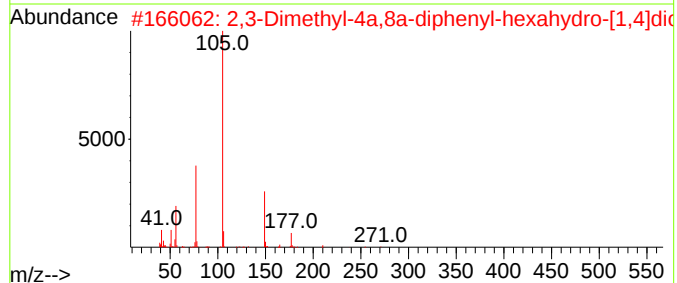
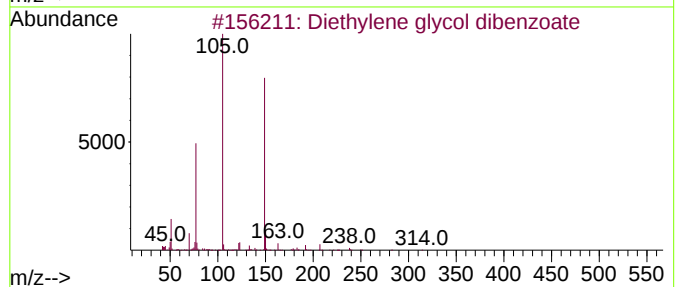
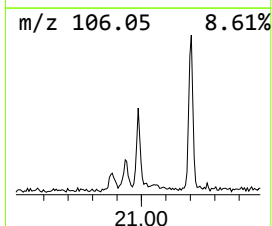
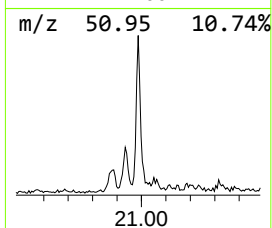
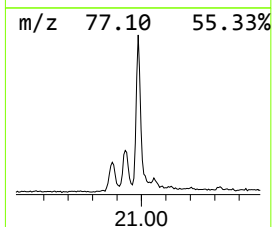
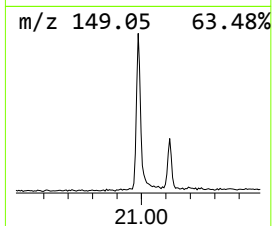
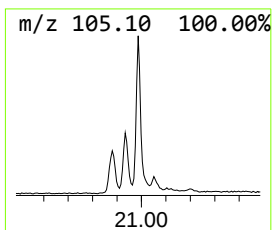
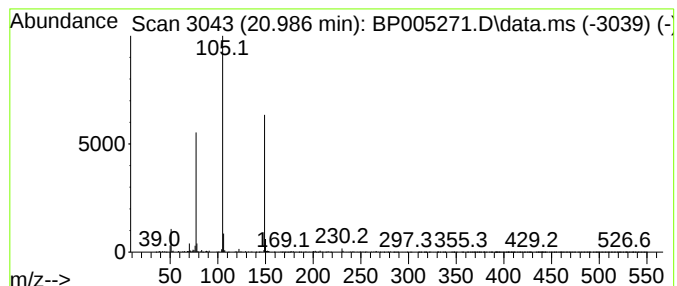
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	7.66 ng	256935	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2			2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56
5			S-Triazine, 1,3,5-tribenzoylhexa...	399	C24H21N3O3	005434-82-2	47



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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-...	4.817	38.5	ng	439085	1	7.675	227840	20.0
Indole	11.981	4.5	ng	59714	2	10.469	266157	20.0
2-Pentadecanone...	17.198	3.1	ng	68878	4	17.098	446434	20.0
Cyclotetradecane	20.922	8.1	ng	271113	5	21.204	671173	20.0
Diethylene glyc...	20.986	7.7	ng	256935	5	21.204	671173	20.0