

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
 Data File : BF130040.D
 Acq On : 29 Aug 2022 18:14
 Operator : CG\JU
 Sample : N4354-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-22

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130040.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.151	308	317	325	rBV2	30630	54820	1.24%	0.224%
2	4.240	325	332	338	rBV2	28758	47728	1.08%	0.195%
3	4.904	443	445	463	rBV	222936	321345	7.28%	1.311%
4	5.340	516	519	541	rBV	1491713	1818550	41.18%	7.420%
5	5.716	580	583	588	rBV	61227	58225	1.32%	0.238%
6	6.369	691	694	709	rBV	1005310	1261981	28.57%	5.149%
7	6.698	747	750	757	rBV	819266	743571	16.84%	3.034%
8	6.875	777	780	787	rVB	379251	321682	7.28%	1.313%
9	6.945	787	792	801	rVV	78557	79466	1.80%	0.324%
10	7.039	805	808	813	rVB2	38933	50150	1.14%	0.205%
11	7.092	813	817	820	rBV	88196	78933	1.79%	0.322%
12	7.228	835	840	843	rBV	58803	57611	1.30%	0.235%
13	7.275	843	848	851	rBV	2583189	2532505	57.34%	10.333%
14	7.469	878	881	883	rBV	195848	156084	3.53%	0.637%
15	7.492	883	885	891	rVB	129365	113051	2.56%	0.461%
16	7.651	910	912	917	rVB2	55222	68664	1.55%	0.280%
17	7.716	919	923	926	rBV	169608	152149	3.44%	0.621%
18	7.816	938	940	943	rBV	56886	48731	1.10%	0.199%
19	7.981	961	968	974	rBV	1097523	1240758	28.09%	5.063%
20	8.281	1012	1019	1026	rBV7	30016	88597	2.01%	0.362%
21	8.445	1039	1047	1050	rBV2	37838	58709	1.33%	0.240%
22	8.728	1092	1095	1101	rBV	50309	65709	1.49%	0.268%
23	8.792	1101	1106	1115	rVB	184463	227770	5.16%	0.929%
24	9.057	1146	1151	1154	rBV	4726928	4416608	100.00%	18.021%
25	9.339	1194	1199	1206	rBV	62559	75924	1.72%	0.310%
26	9.733	1262	1266	1270	rBV	1385343	1119356	25.34%	4.567%
27	10.122	1330	1332	1336	rVB	75226	65447	1.48%	0.267%
28	10.533	1398	1402	1405	rBV	3258083	2744280	62.14%	11.197%
29	10.963	1472	1475	1485	rBV	33058	49221	1.11%	0.201%
30	11.222	1516	1519	1523	rBV	1163229	1027165	23.26%	4.191%
31	11.751	1606	1609	1618	rBV3	113744	144236	3.27%	0.589%
32	12.810	1784	1789	1792	rBV	4120660	3707235	83.94%	15.127%
33	12.945	1806	1812	1814	rBV4	24031	45759	1.04%	0.187%
34	13.751	1945	1949	1955	rBV5	42431	89074	2.02%	0.363%
35	13.868	1966	1969	1973	rBV	674132	583971	13.22%	2.383%
36	14.104	2007	2009	2016	rVB5	27107	46418	1.05%	0.189%

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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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.674	2103	2106	2111	rVB	59300	58018	1.31%	0.237%
38	15.298	2208	2212	2222	rVB	546987	688641	15.59%	2.810%

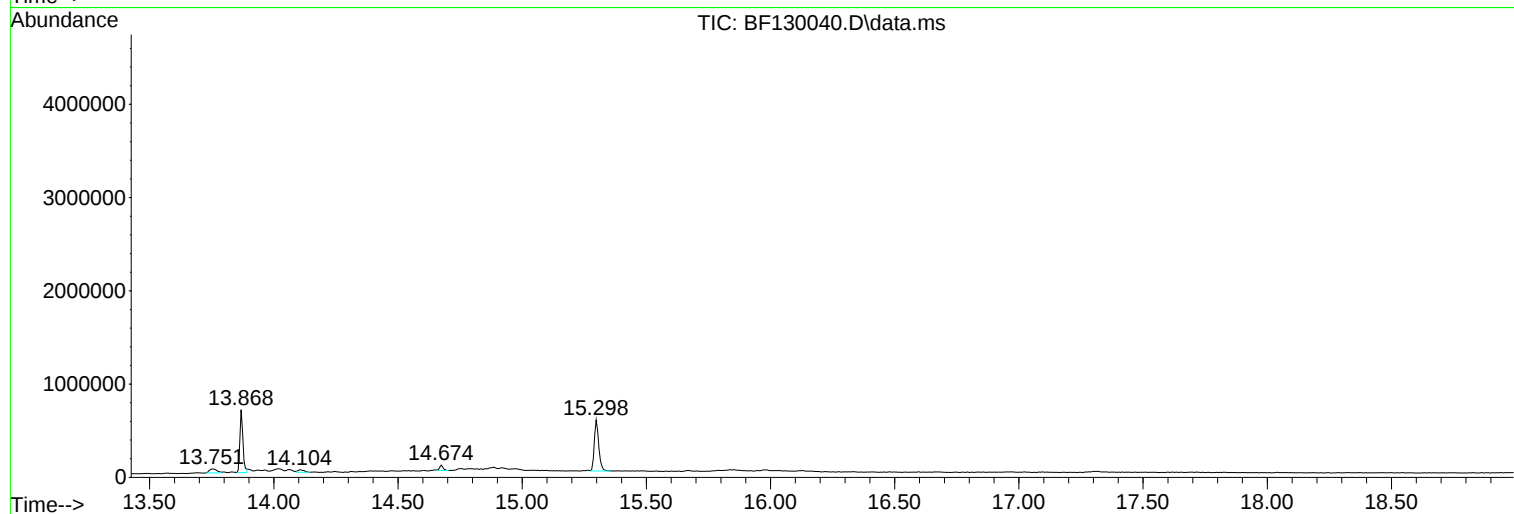
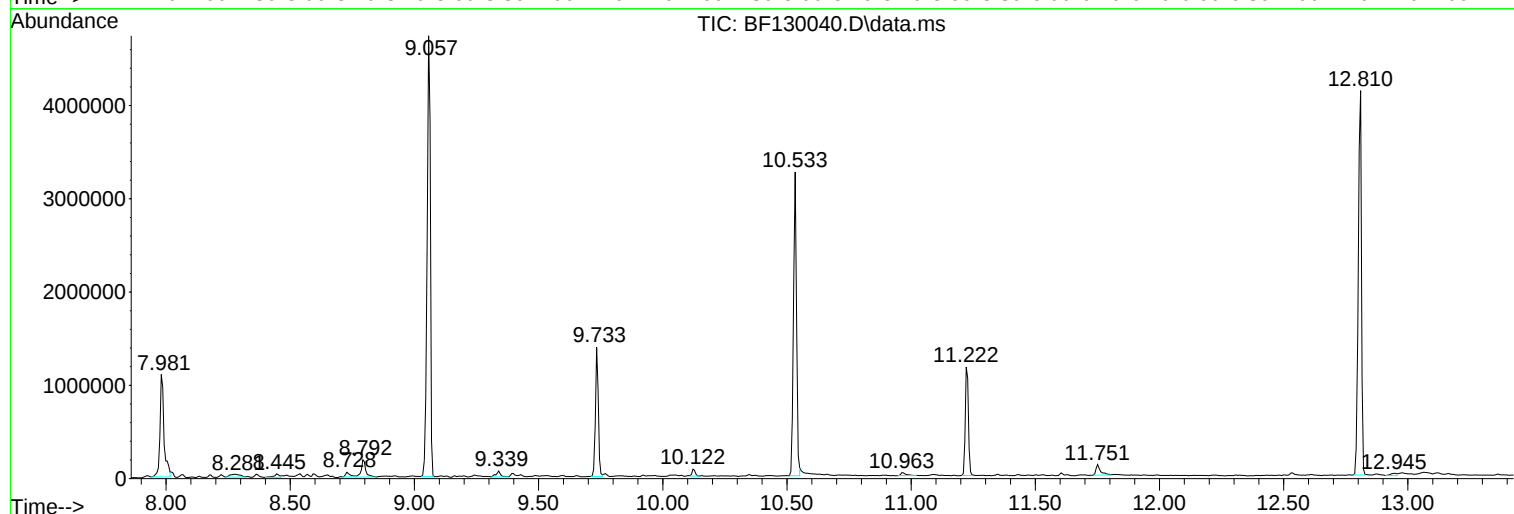
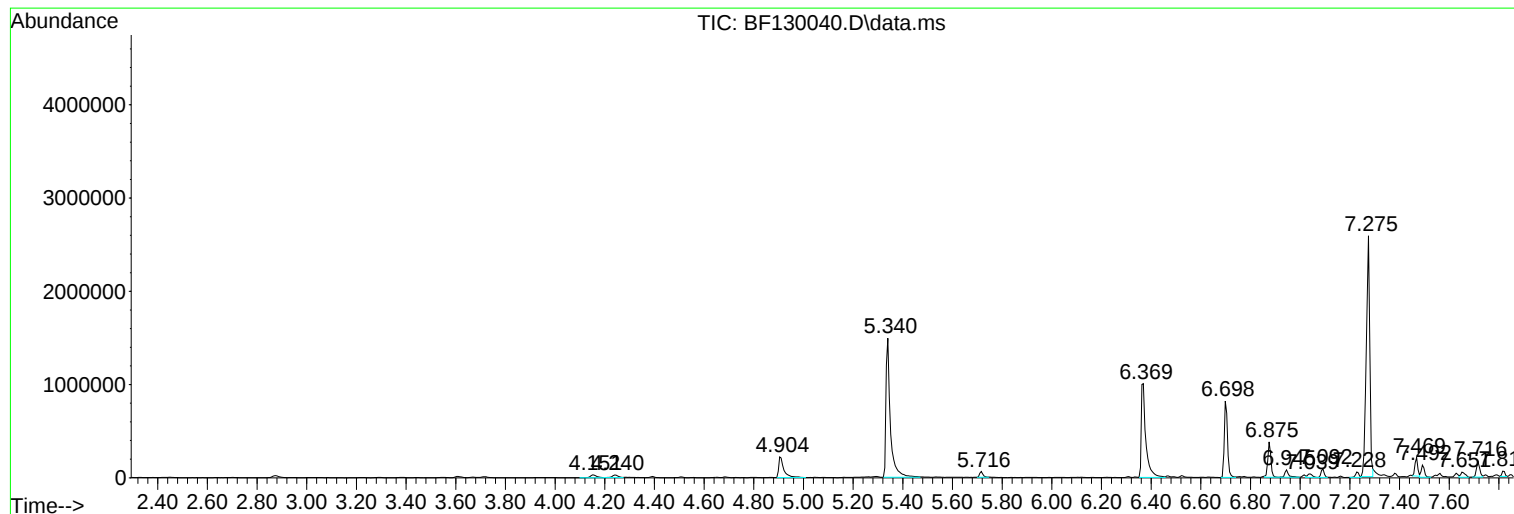
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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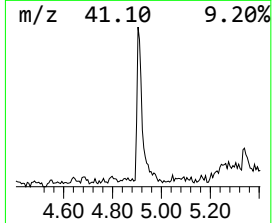
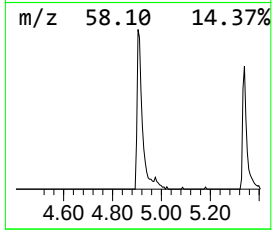
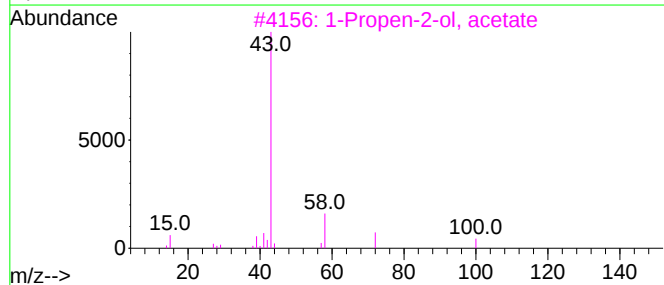
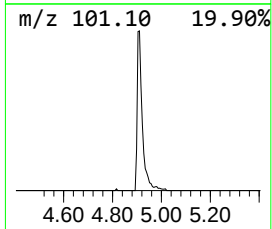
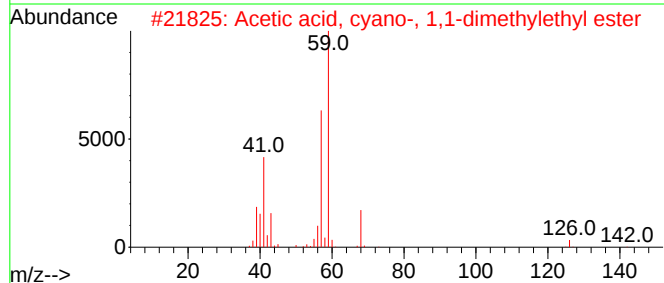
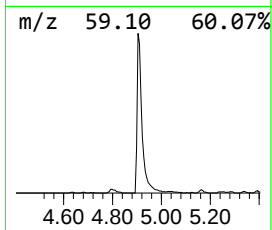
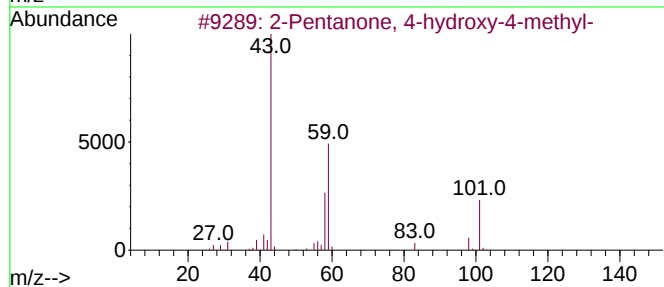
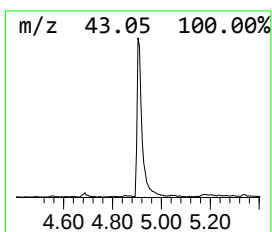
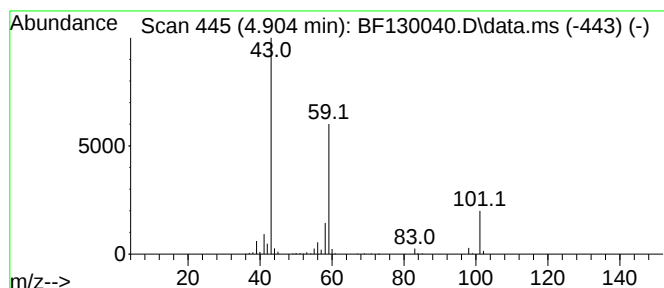
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	8.64 ng	321345	1,4-Dichlorobenzene-d4	6.698

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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ClientSampleId :
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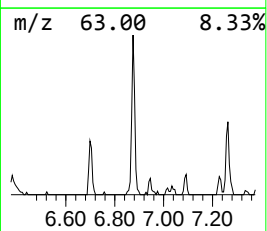
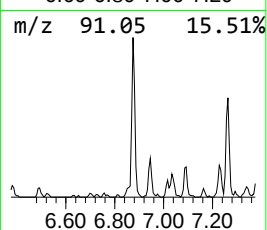
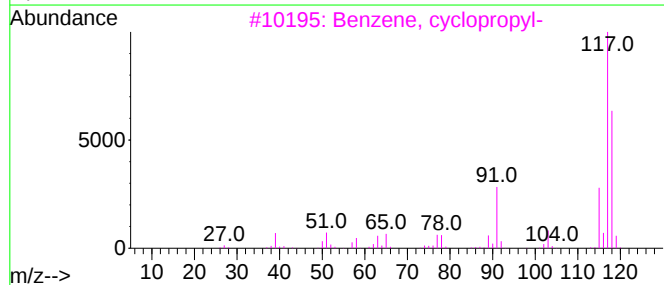
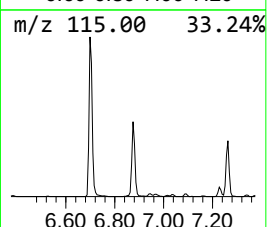
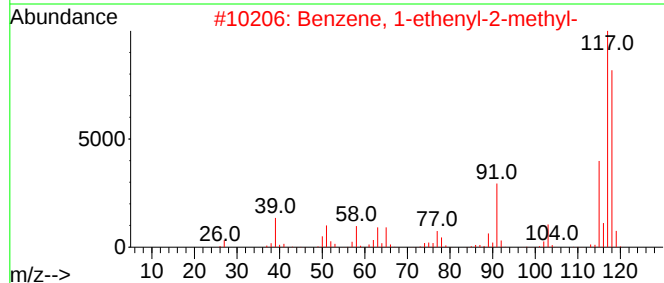
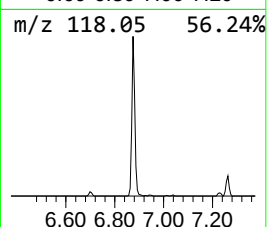
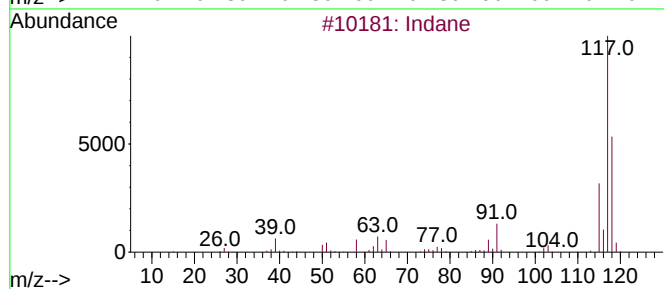
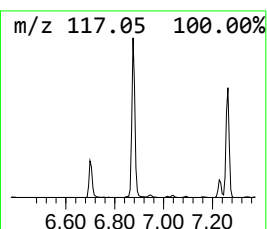
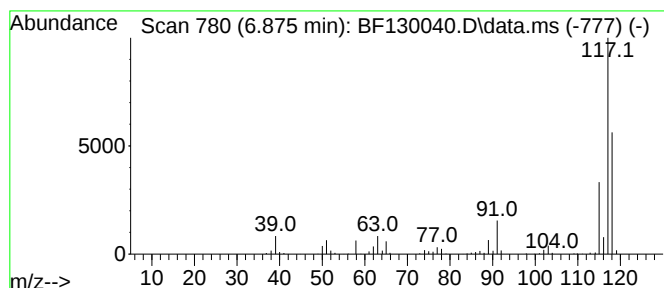
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.875	8.65 ng	321682	1,4-Dichlorobenzene-d4	6.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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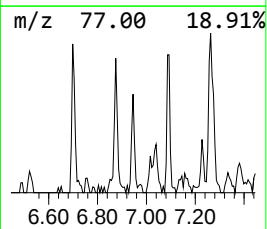
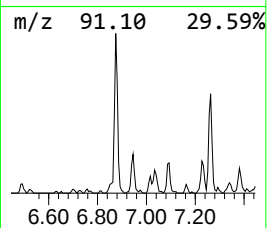
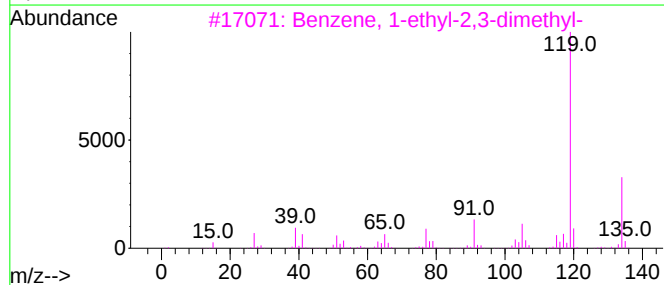
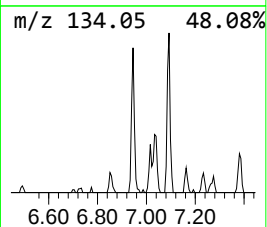
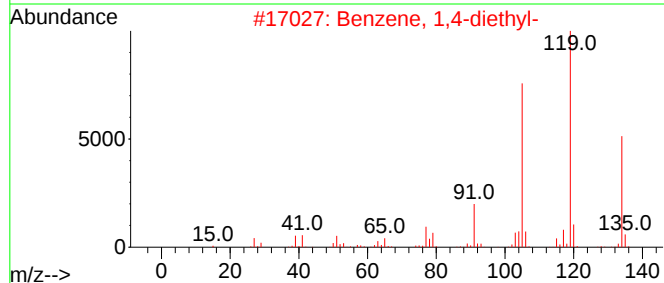
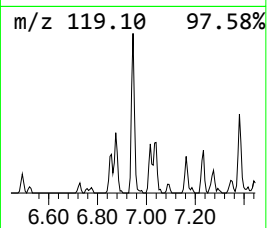
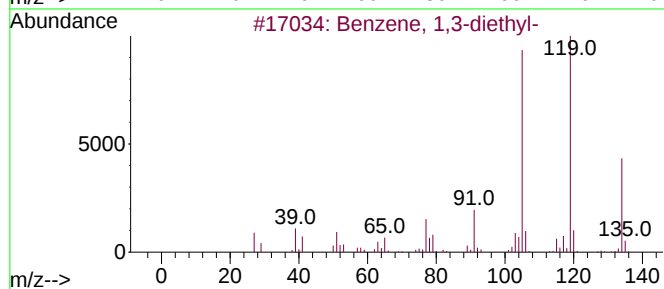
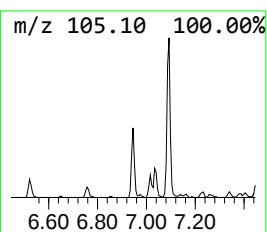
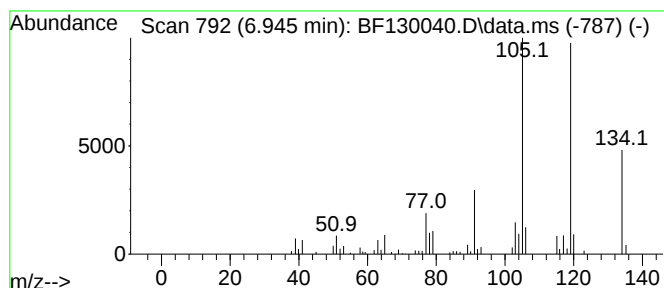
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1,3-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.945	2.14 ng	79466	1,4-Dichlorobenzene-d4	6.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	91
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	90



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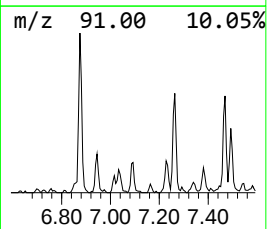
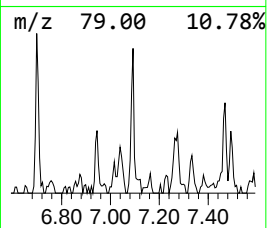
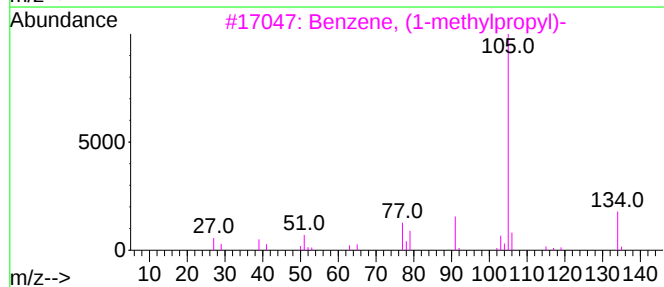
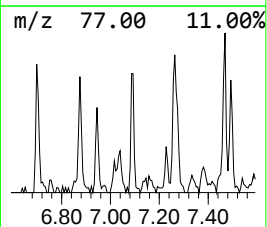
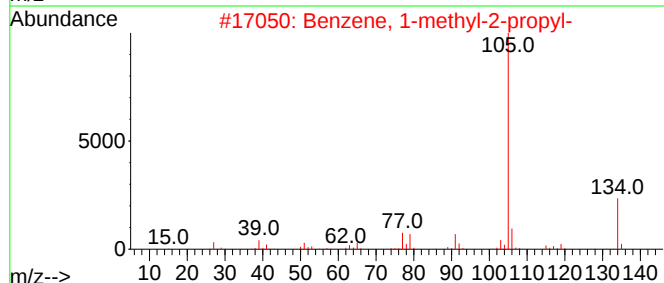
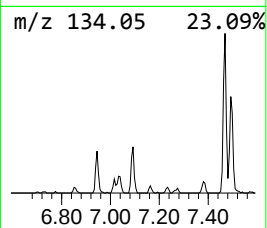
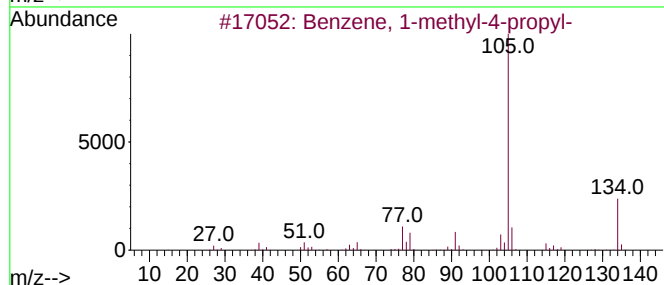
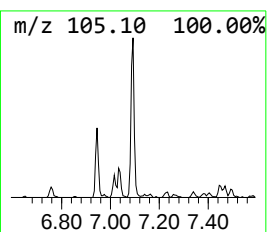
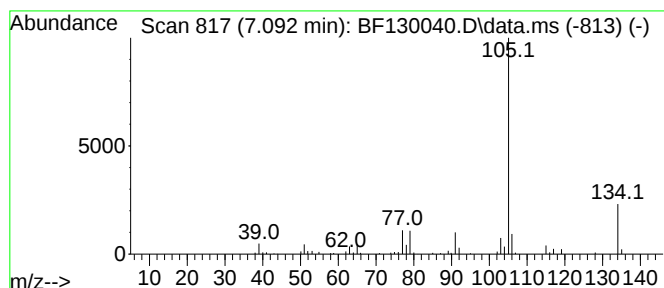
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-methyl-4-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.092	2.12 ng	78933	1,4-Dichlorobenzene-d4	6.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	95
2			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91
3			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	91
4			Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	90
5			Oxirane, 2-methyl-2-phenyl-	134	C9H10O	002085-88-3	86



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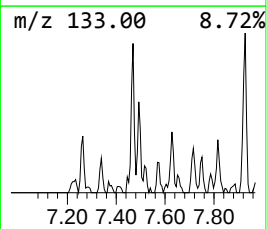
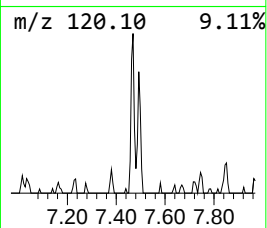
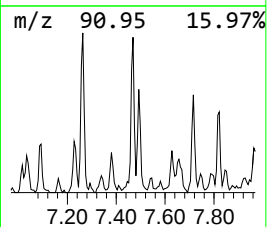
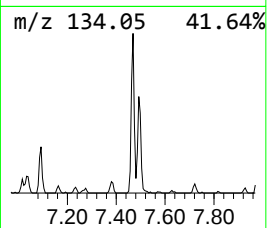
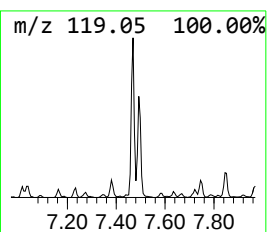
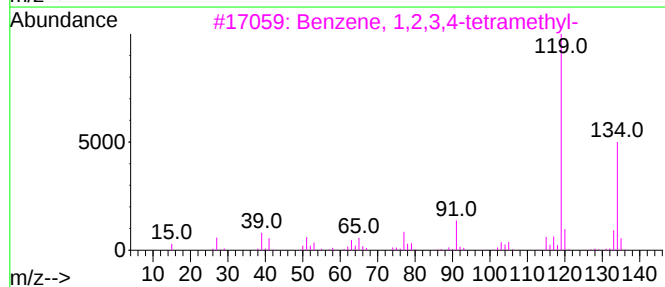
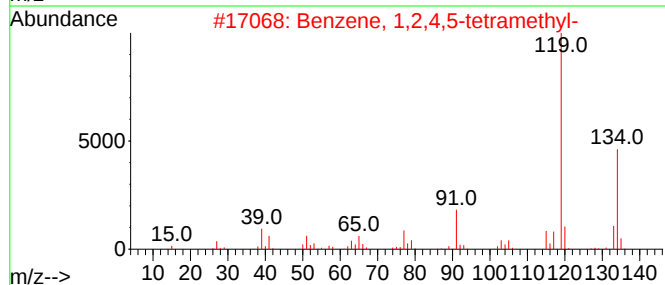
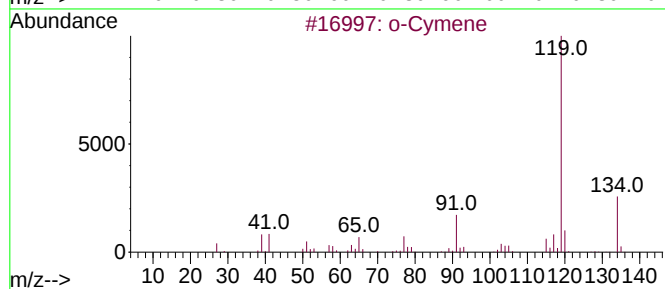
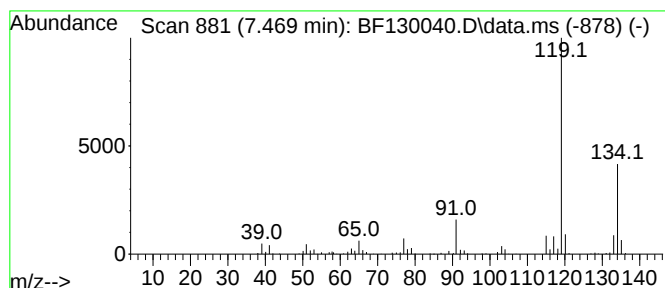
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.469	2.52 ng	156084	Naphthalene-d8	7.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	96
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130040.D
Acq On : 29 Aug 2022 18:14
Operator : CG\JU
Sample : N4354-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-22

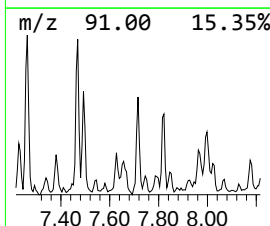
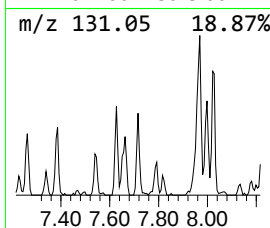
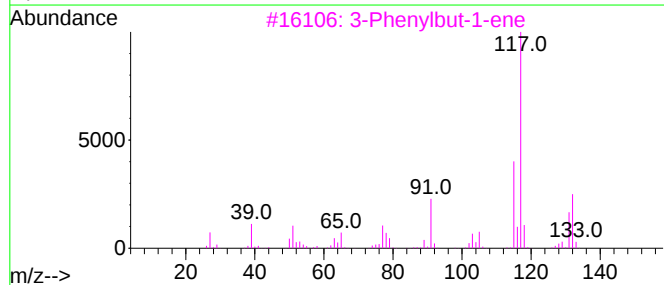
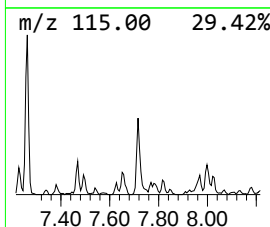
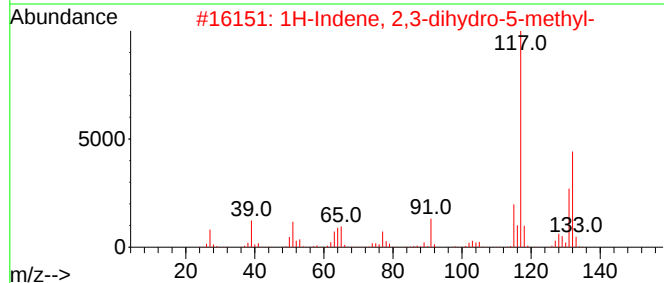
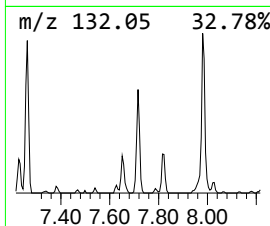
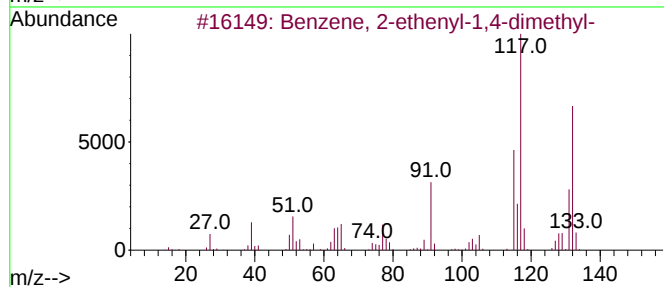
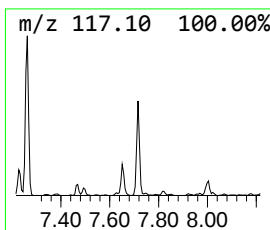
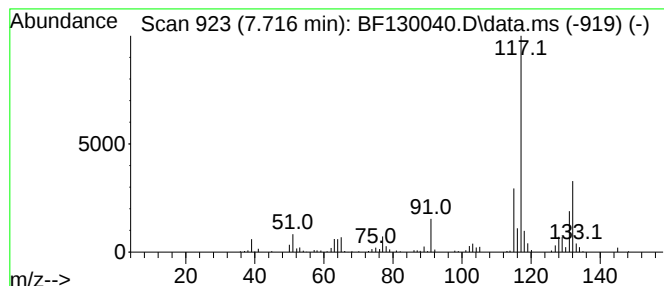
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.716	2.45 ng	152149	Naphthalene-d8	7.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130040.D
Acq On : 29 Aug 2022 18:14
Operator : CG\JU
Sample : N4354-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

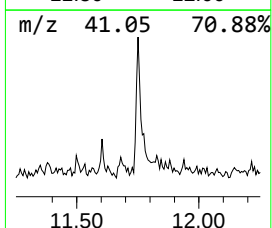
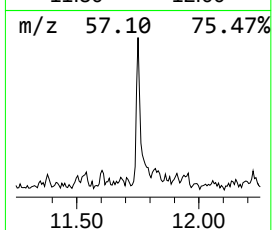
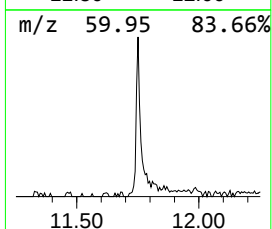
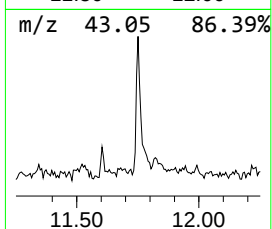
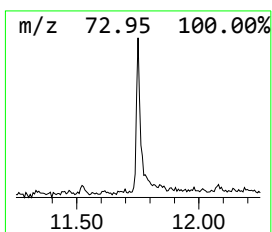
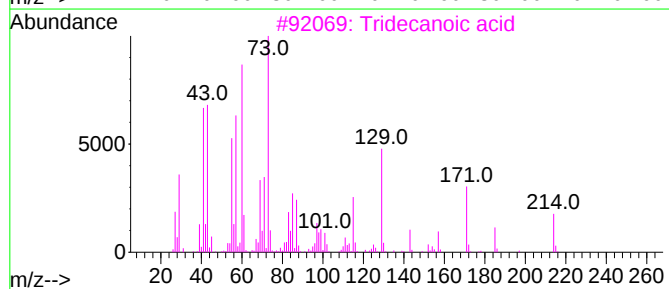
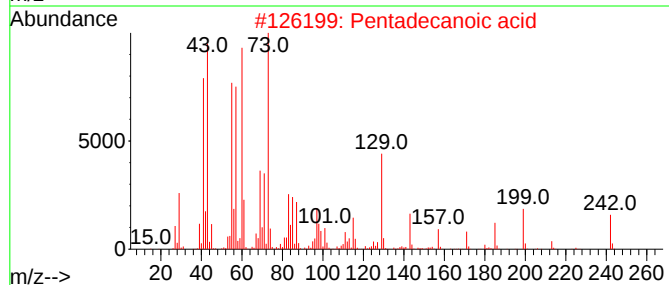
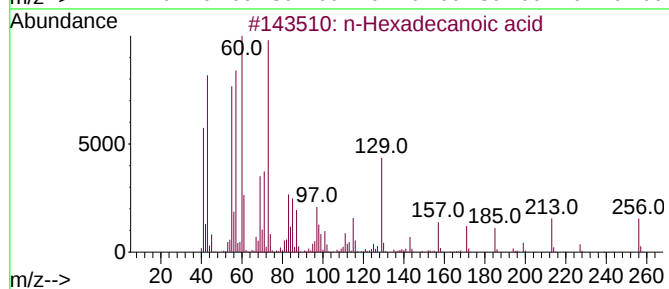
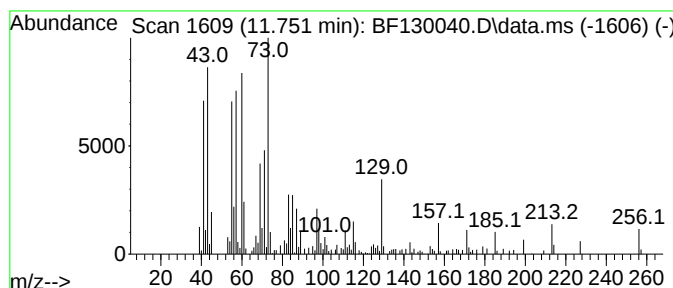
Instrument :
BNA_F
ClientSampleId :
MW-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.751	2.81 ng	144236	Phenanthrene-d10	11.222	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130040.D
Acq On : 29 Aug 2022 18:14
Operator : CG\JU
Sample : N4354-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

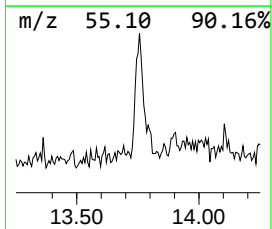
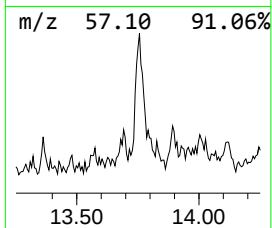
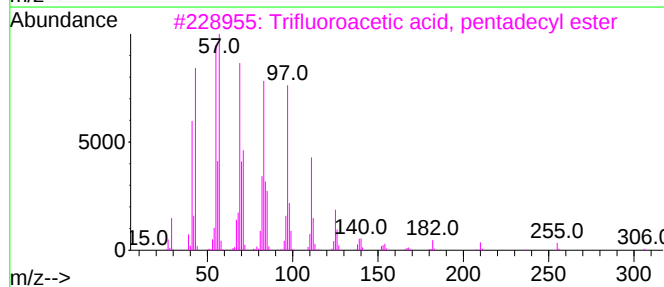
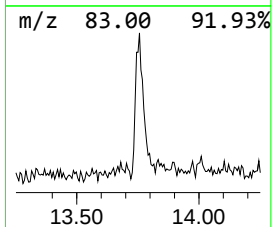
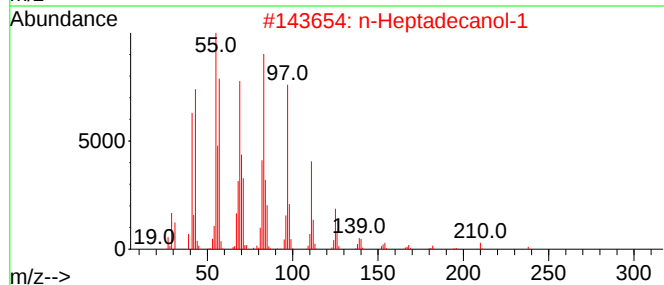
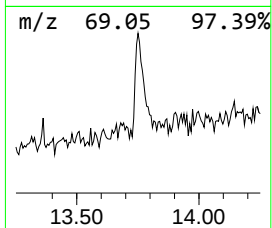
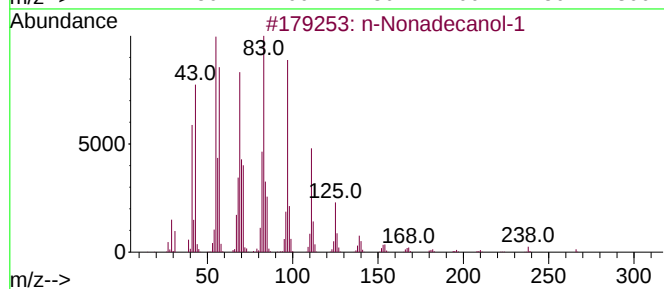
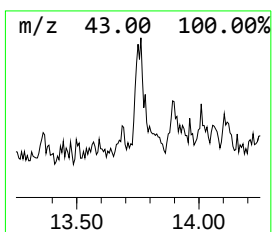
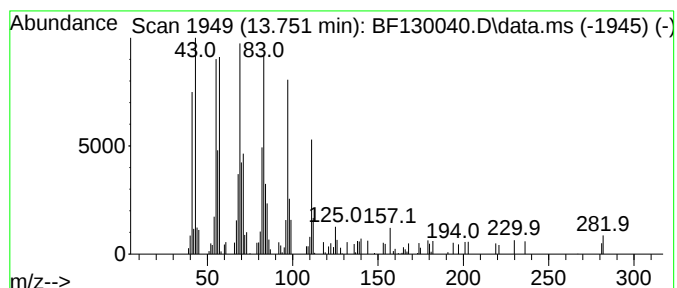
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.751	3.05 ng	89074	Chrysene-d12	13.868	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	n-Pentadecanol	228	C15H32O	000629-76-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130040.D
Acq On : 29 Aug 2022 18:14
Operator : CG\JU
Sample : N4354-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Indane	6.875	8.7	ng	321682	1	6.698	743571	20.0
Benzene, 1,3-di...	6.945	2.1	ng	79466	1	6.698	743571	20.0
Benzene, 1-meth...	7.092	2.1	ng	78933	1	6.698	743571	20.0
o-Cymene	7.469	2.5	ng	156084	2	7.981	1240760	20.0
Benzene, 2-ethe...	7.716	2.5	ng	152149	2	7.981	1240760	20.0
n-Hexadecanoic ...	11.751	2.8	ng	144236	4	11.222	1027170	20.0
n-Nonadecanol-1	13.751	3.0	ng	89074	5	13.868	583971	20.0