

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
 Data File : BP008099.D
 Acq On : 23 Nov 2021 16:47
 Operator : CG/JU
 Sample : M4808-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CHRT-20001

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-BP111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.022	3	6	13	rBV	774206	1021554	17.34%	2.339%
2	4.946	327	333	339	rBV	428158	607792	10.32%	1.392%
3	5.411	405	412	433	rBV	2303022	3427851	58.20%	7.849%
4	6.999	673	682	698	rBV	2195848	3720489	63.16%	8.519%
5	7.822	813	822	830	rBV	547499	877787	14.90%	2.010%
6	8.981	1008	1019	1029	rBV	1504731	2487963	42.24%	5.697%
7	10.410	1254	1262	1271	rBV2	44393	93929	1.59%	0.215%
8	10.616	1287	1297	1305	rBV	745461	1330528	22.59%	3.047%
9	11.663	1470	1475	1480	rBV6	42276	106848	1.81%	0.245%
10	12.363	1589	1594	1600	rBV7	60395	124544	2.11%	0.285%
11	12.540	1620	1624	1628	rBV3	101166	160466	2.72%	0.367%
12	12.904	1683	1686	1691	rVB3	117926	168380	2.86%	0.386%
13	12.963	1692	1696	1701	rVV6	89316	180795	3.07%	0.414%
14	13.010	1701	1704	1708	rVB	154932	191190	3.25%	0.438%
15	13.087	1709	1717	1726	rVV	3510066	5437746	92.32%	12.452%
16	13.245	1742	1744	1748	rBV2	127186	151550	2.57%	0.347%
17	13.298	1750	1753	1759	rVB2	164565	218376	3.71%	0.500%
18	13.740	1825	1828	1832	rBV5	222732	295037	5.01%	0.676%
19	13.816	1838	1841	1849	rVB2	426925	693484	11.77%	1.588%
20	13.887	1849	1853	1857	rBV	506068	707228	12.01%	1.619%
21	13.963	1862	1866	1869	rBV3	382470	517876	8.79%	1.186%
22	14.298	1919	1923	1931	rVB4	914383	1712905	29.08%	3.922%
23	14.375	1932	1936	1941	rBV4	420381	665803	11.30%	1.525%
24	14.463	1942	1951	1955	rBV3	1354574	3439587	58.39%	7.876%
25	14.998	2040	2042	2050	rVB6	514130	746873	12.68%	1.710%
26	15.263	2083	2087	2091	rBV2	938478	1380723	23.44%	3.162%
27	15.963	2202	2206	2210	rBV2	2030412	3085198	52.38%	7.065%
28	19.798	2854	2858	2865	rVB	4733312	5890225	100.00%	13.488%
29	21.322	3114	3117	3134	rVB	1402794	2523717	42.85%	5.779%
30	23.721	3519	3525	3533	rVB2	812593	1703872	28.93%	3.902%

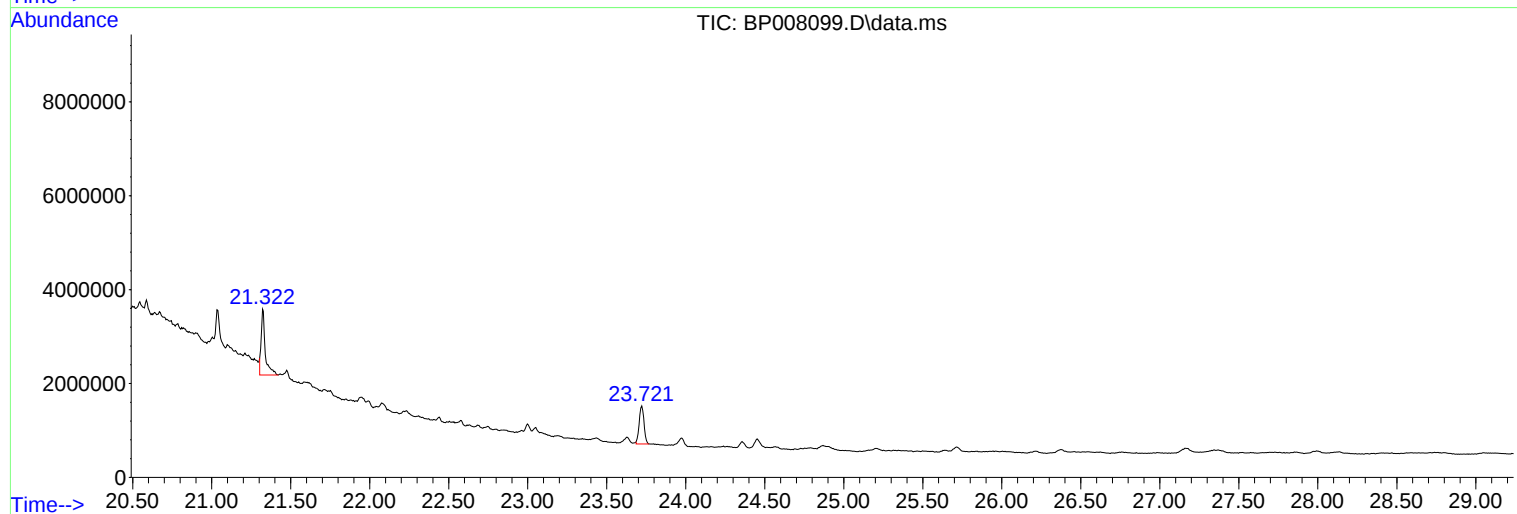
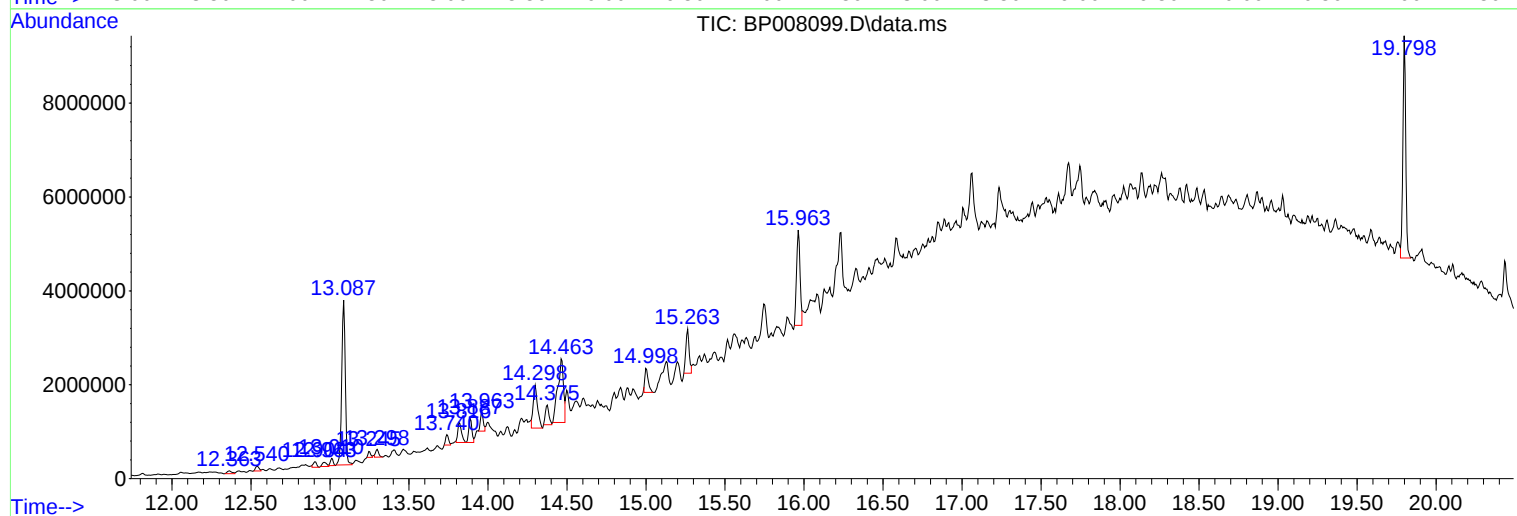
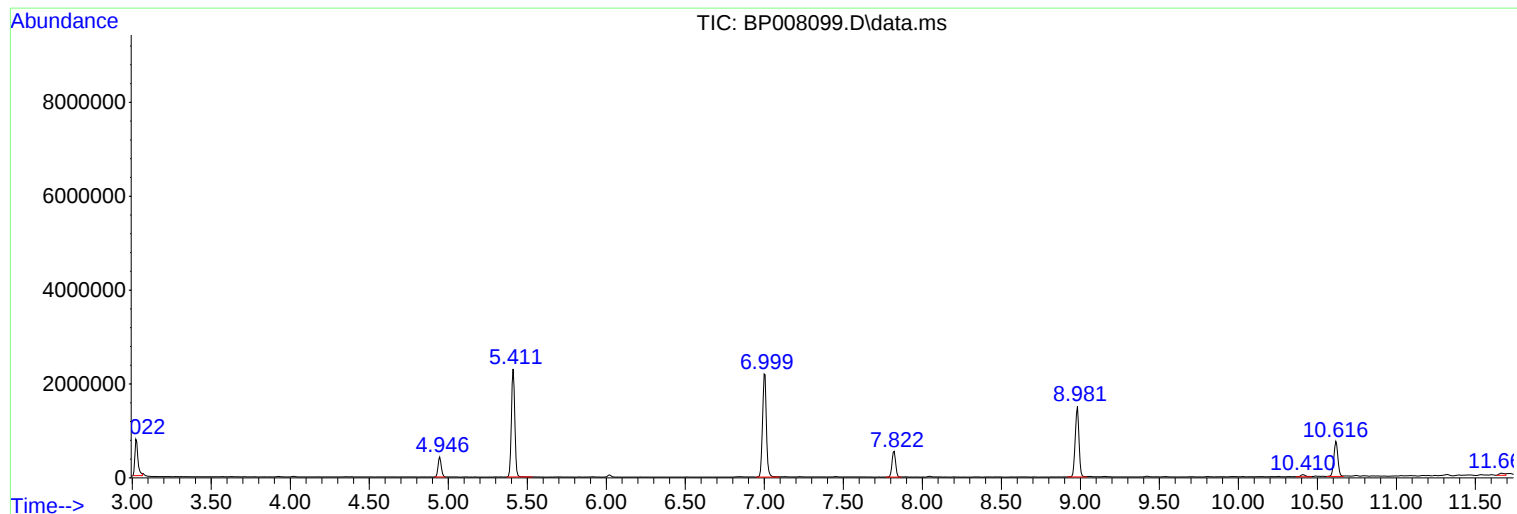
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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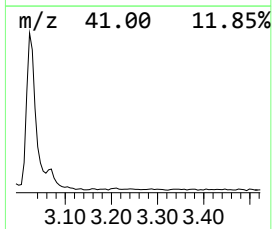
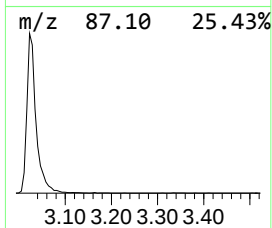
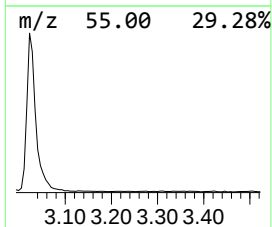
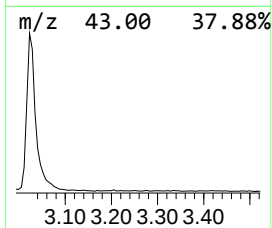
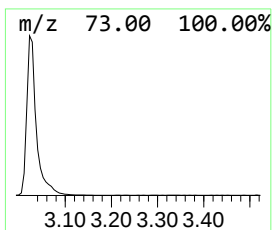
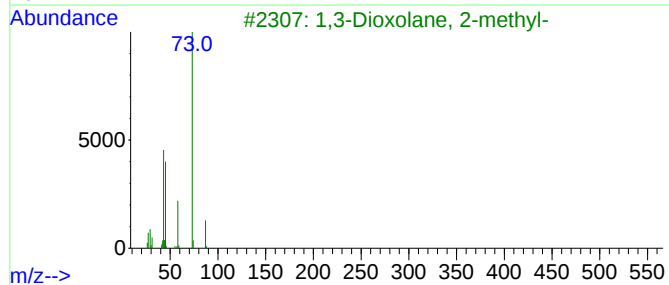
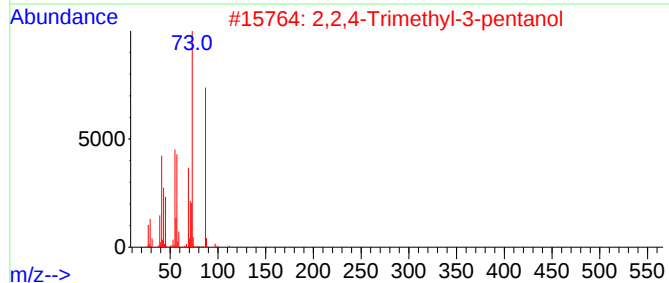
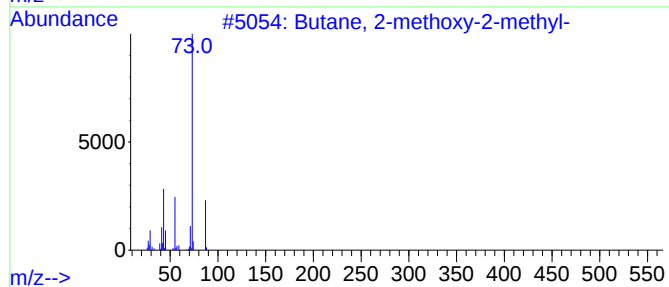
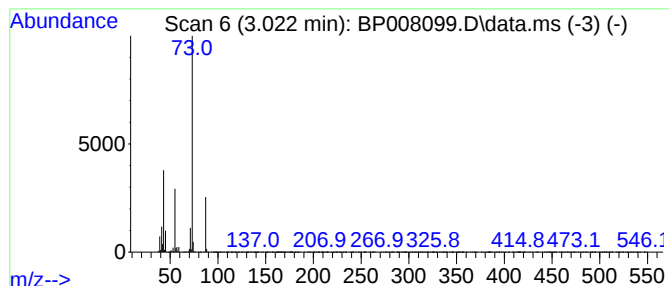
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.022	23.28 ng	1021550	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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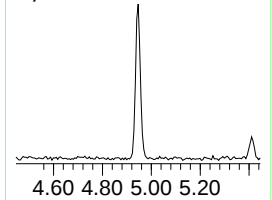
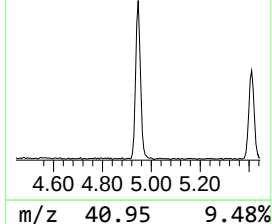
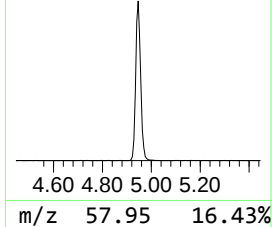
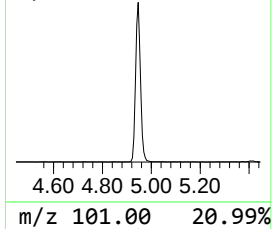
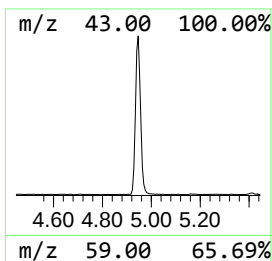
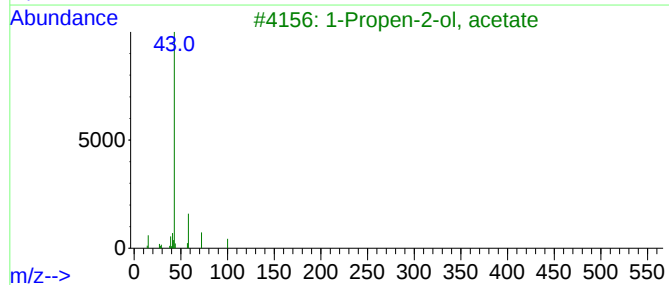
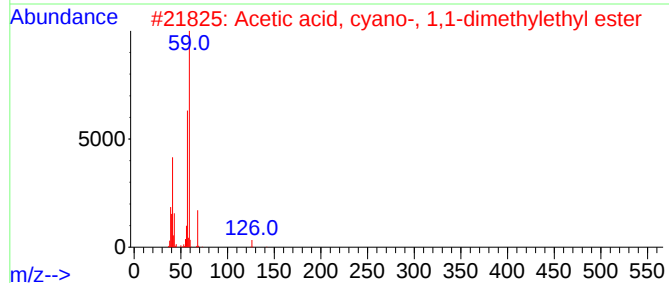
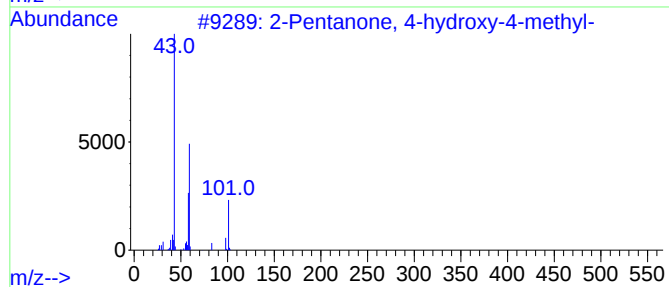
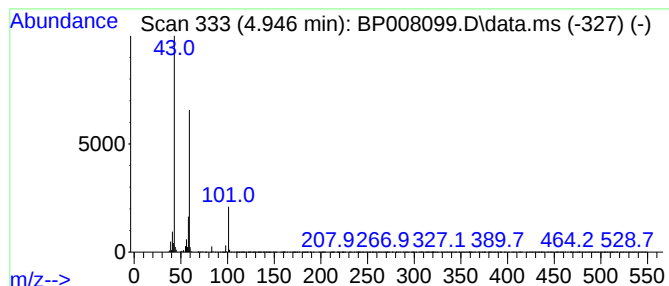
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	13.85 ng	607792	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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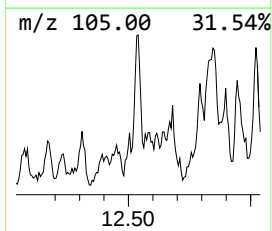
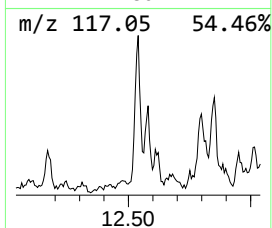
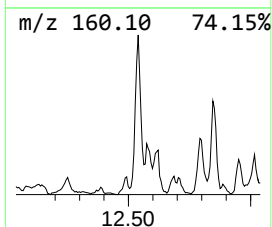
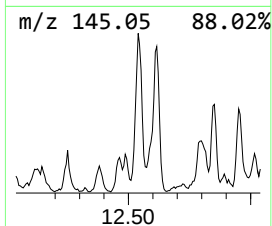
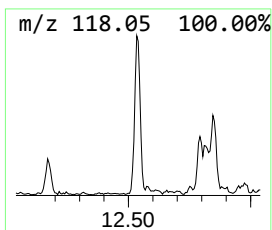
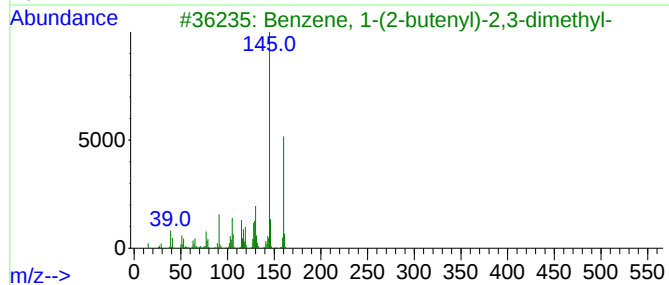
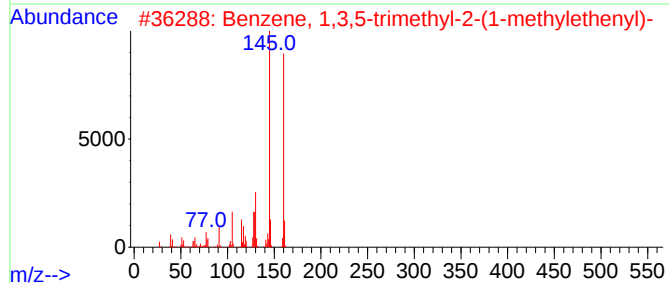
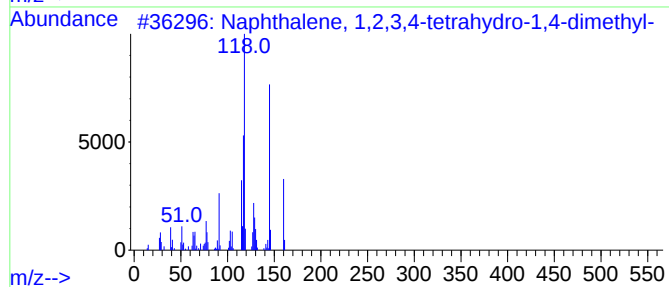
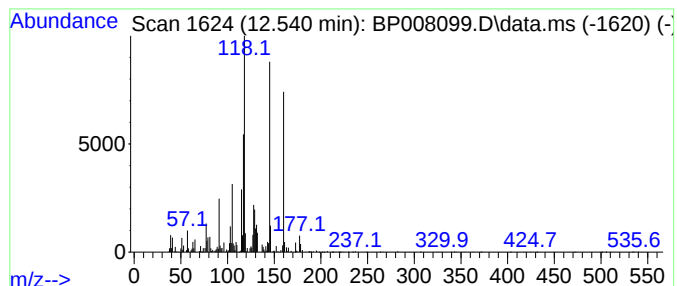
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.540	2.41 ng	160466	Naphthalene-d8	10.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	78
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	64
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	64
5	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	62



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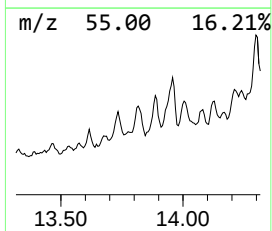
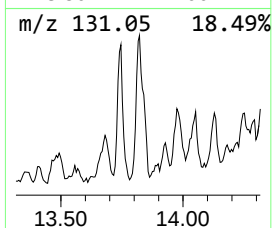
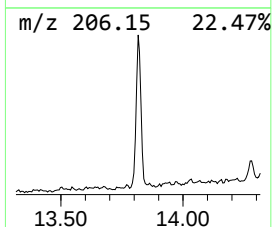
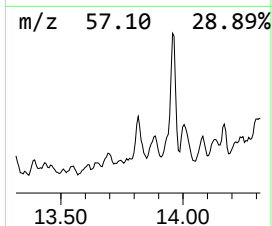
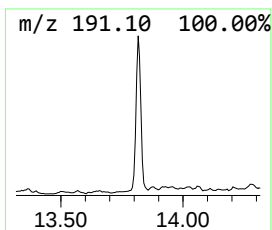
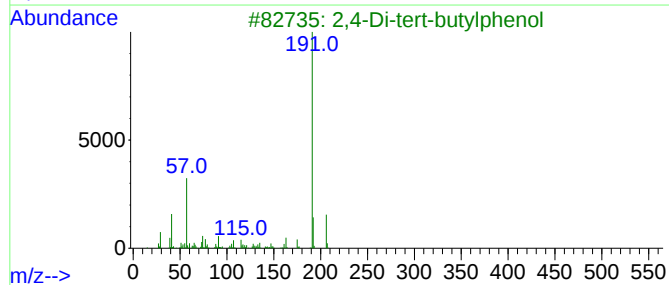
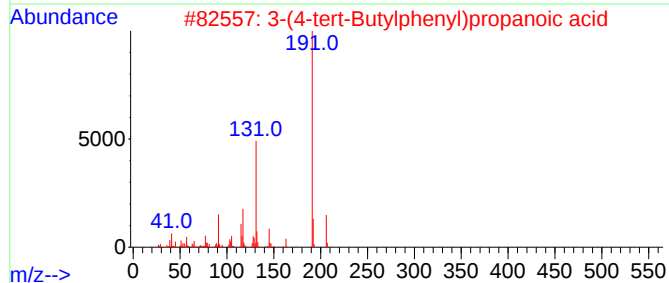
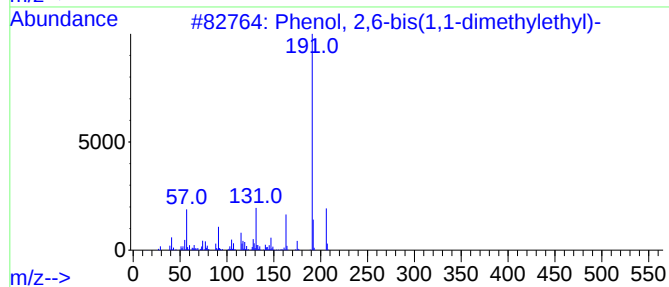
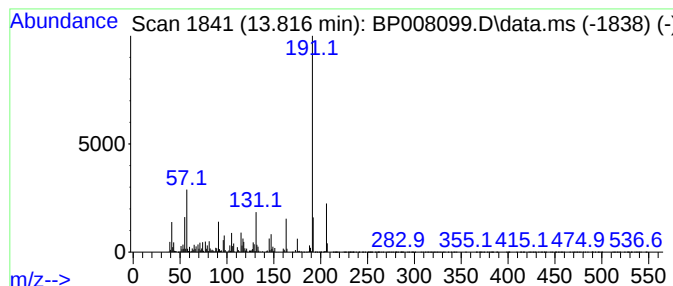
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Peak Number 4 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	4.03 ng	693484	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	87
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
4			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	80
5			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	80



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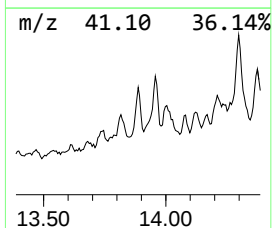
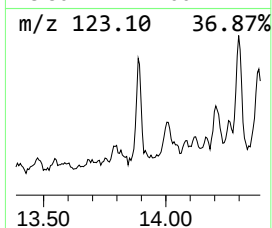
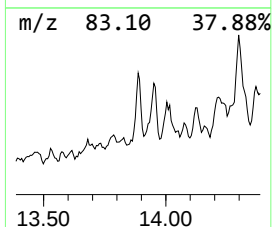
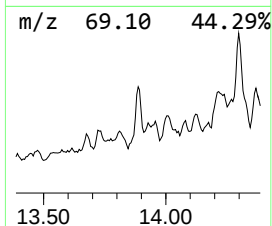
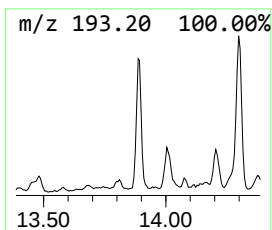
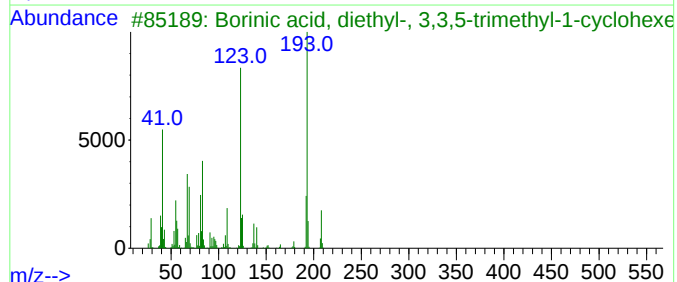
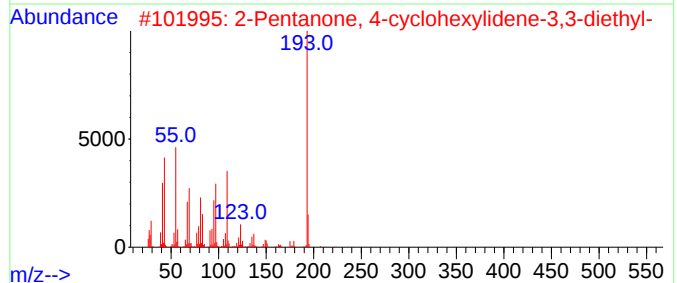
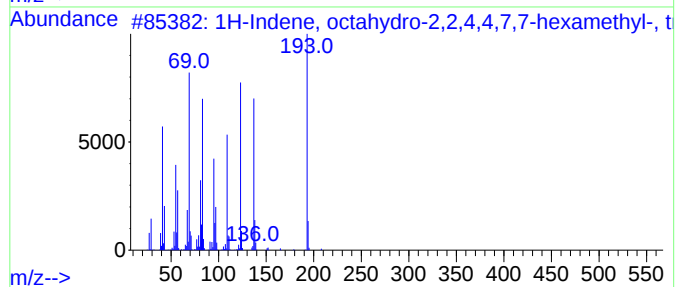
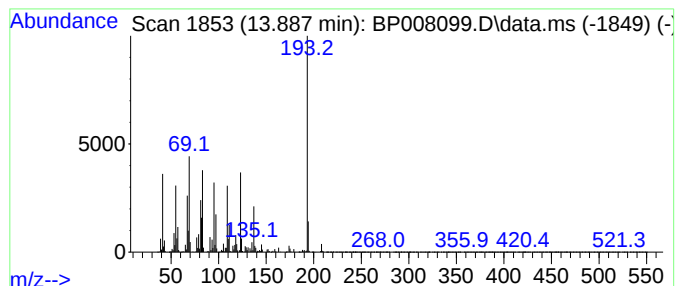
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Peak Number 5 1H-Indene, octahydro-2,2,4,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.887	4.11 ng	707228	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
3			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
4			Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	35
5			[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	30



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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-20001

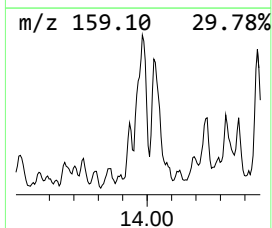
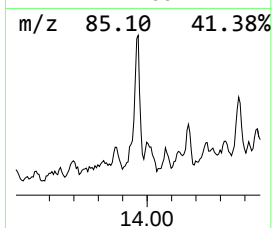
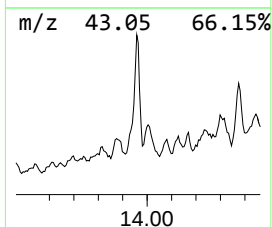
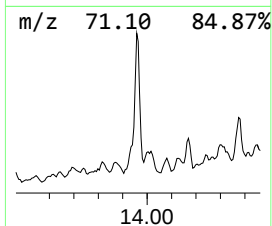
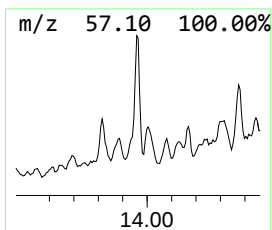
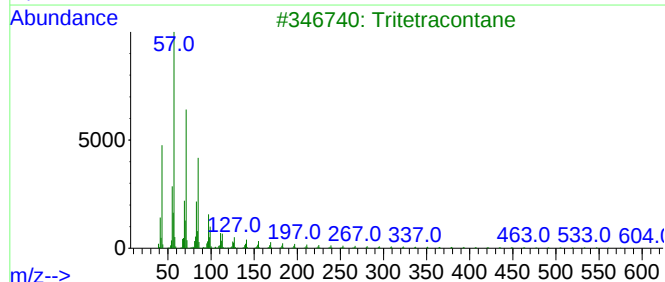
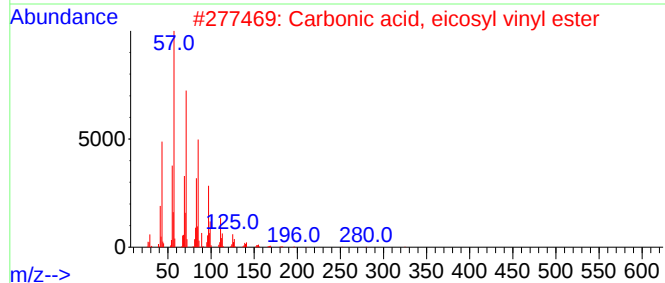
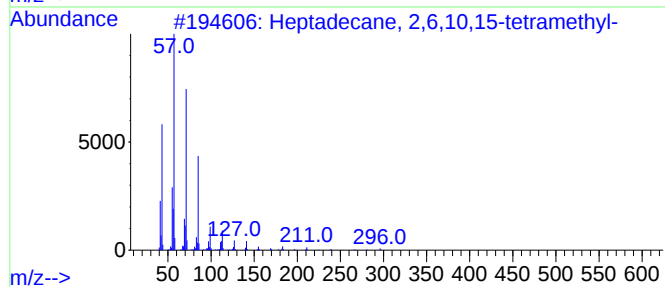
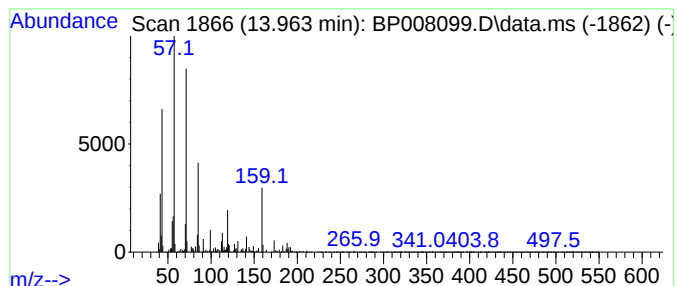
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	3.01 ng	517876	Acenaphthene-d10	14.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	68
2		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	58
3		Tritetracontane	605	C43H88	007098-21-7	53
4		Tridecane, 4-methyl-	198	C14H30	026730-12-1	53
5		1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008099.D
Acq On : 23 Nov 2021 16:47
Operator : CG/JU
Sample : M4808-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-20001

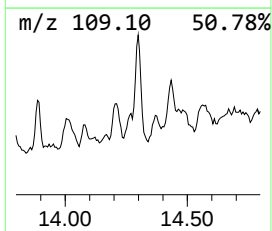
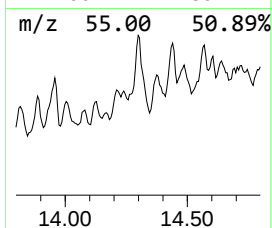
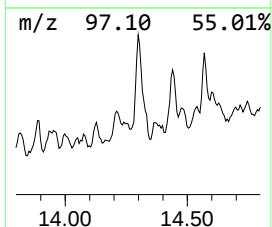
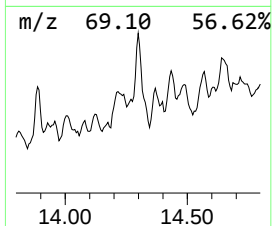
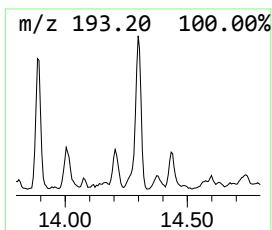
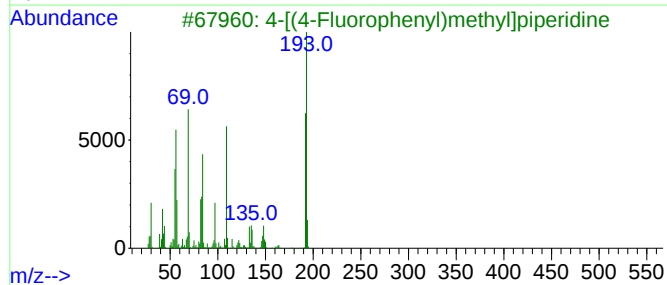
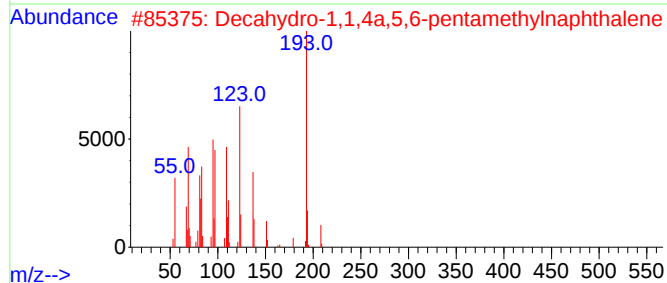
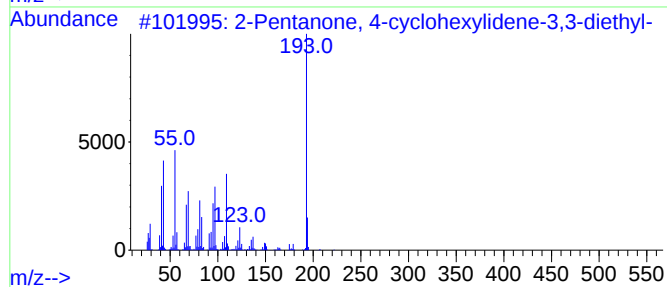
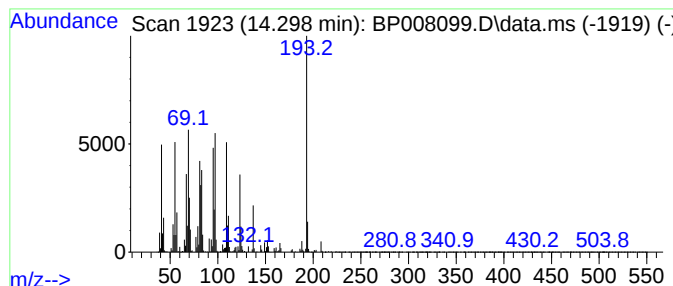
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Pentanone, 4-cyclohexylidene-3,3-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.298	9.96 ng	1712910	Acenaphthene-d10	14.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	53	
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43	
3	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	38	
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38	
5	Benzenamine, 4-(hexyloxy)-	193	C12H19NO	039905-57-2	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008099.D
Acq On : 23 Nov 2021 16:47
Operator : CG/JU
Sample : M4808-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-20001

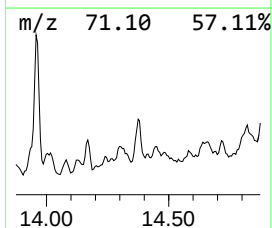
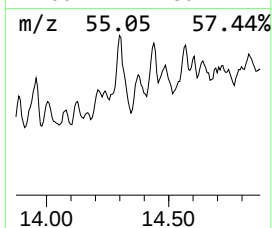
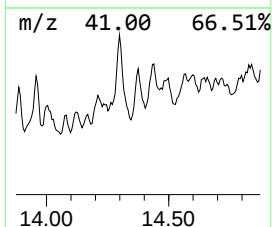
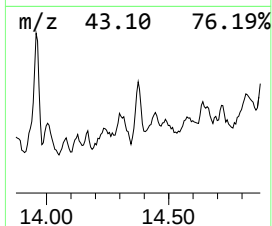
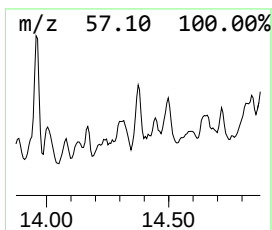
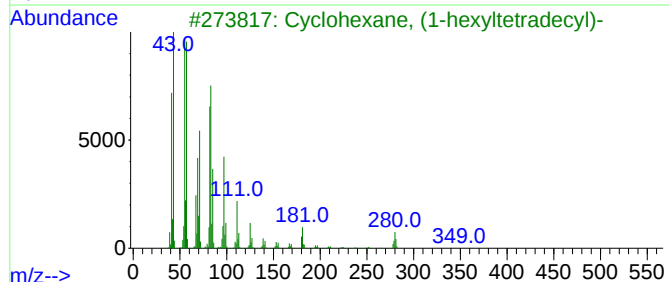
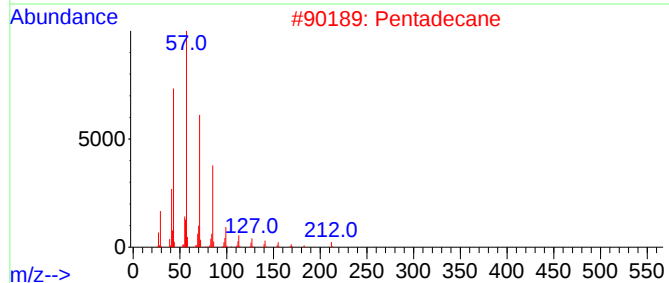
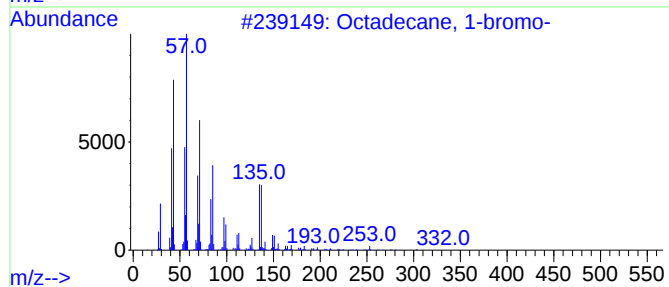
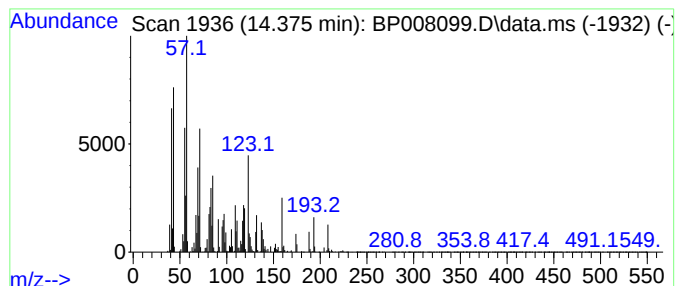
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.375 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.375	3.87 ng	665803	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	25
2			Pentadecane	212	C15H32	000629-62-9	25
3			Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	15
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	15
5			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008099.D
Acq On : 23 Nov 2021 16:47
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Sample : M4808-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

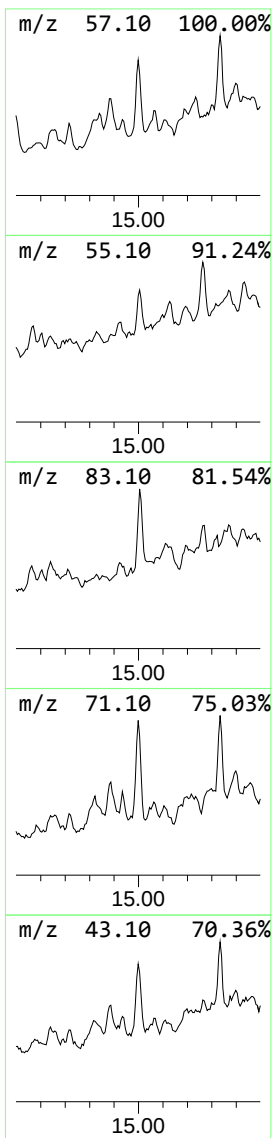
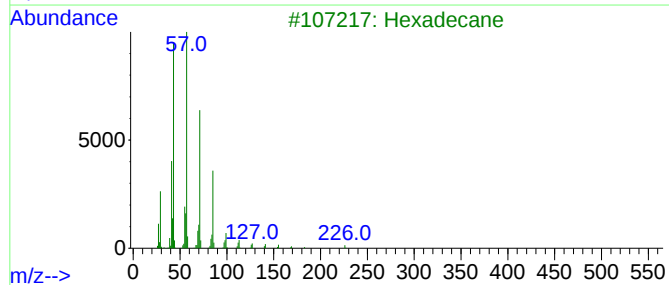
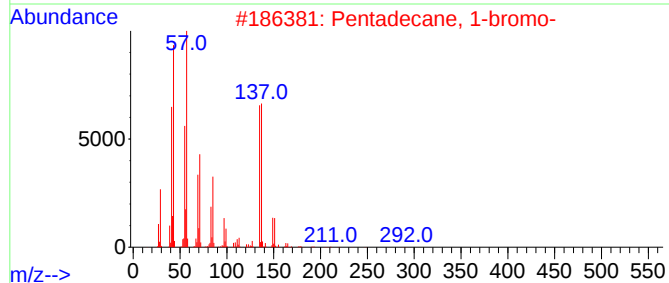
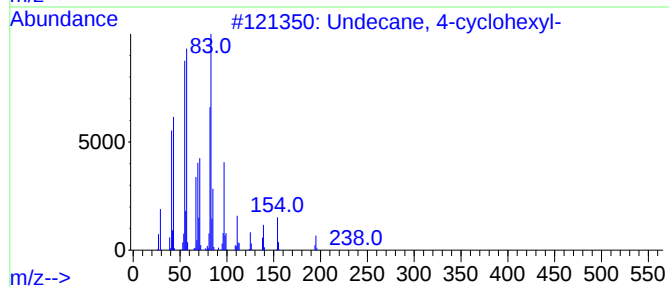
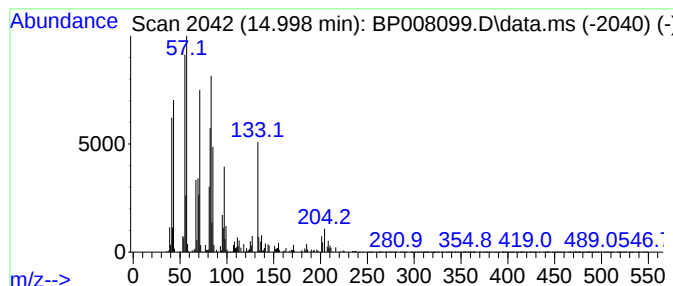
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Undecane, 4-cyclohexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.998	4.34 ng	746873	Acenaphthene-d10		14.463	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Undecane, 4-cyclohexyl-		238	C17H34	013151-79-6	55
2	Pentadecane, 1-bromo-		290	C15H31Br	000629-72-1	46
3	Hexadecane		226	C16H34	000544-76-3	38
4	Dodecane, 4-methyl-		184	C13H28	006117-97-1	30
5	Tritetracontane		605	C43H88	007098-21-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008099.D
Acq On : 23 Nov 2021 16:47
Operator : CG/JU
Sample : M4808-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-20001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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
Butane, 2-metho...	3.022	23.3	ng	1021550	1	7.822	877787	20.0
2-Pentanone, 4-...	4.946	13.9	ng	607792	1	7.822	877787	20.0
Naphthalene, 1,...	12.540	2.4	ng	160466	2	10.616	1330530	20.0
Phenol, 2,6-bis...	13.816	4.0	ng	693484	3	14.463	3439590	20.0
1H-Indene, octa...	13.887	4.1	ng	707228	3	14.463	3439590	20.0
Heptadecane, 2,...	13.963	3.0	ng	517876	3	14.463	3439590	20.0
2-Pentanone, 4-...	14.298	10.0	ng	1712910	3	14.463	3439590	20.0
unknown14.375	14.375	3.9	ng	665803	3	14.463	3439590	20.0
Undecane, 4-cyc...	14.998	4.3	ng	746873	3	14.463	3439590	20.0