

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137063.D
Acq On : 15 Jan 2024 15:11
Operator : CG\JU
Sample : P1132-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200010

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	26	rVB	14329	21287	2.07%	0.244%
2	5.022	495	499	512	rVB	62904	77554	7.54%	0.890%
3	5.434	565	569	589	rBV	921511	844720	82.17%	9.695%
4	6.434	736	739	760	rBV	901880	801079	77.92%	9.194%
5	6.781	795	798	807	rVB	302484	265488	25.83%	3.047%
6	7.345	890	894	897	rBV	632470	500418	48.68%	5.743%
7	8.057	1012	1015	1019	rBV	347631	310075	30.16%	3.559%
8	8.604	1102	1108	1112	rBV7	7781	16084	1.56%	0.185%
9	8.692	1118	1123	1126	rBV7	8659	16518	1.61%	0.190%
10	9.133	1195	1198	1202	rBV	1061443	949619	92.37%	10.898%
11	9.204	1208	1210	1215	rVB5	22366	29192	2.84%	0.335%
12	9.257	1215	1219	1223	rBV6	18374	36594	3.56%	0.420%
13	9.516	1261	1263	1268	rBV4	33563	34995	3.40%	0.402%
14	9.675	1287	1290	1293	rBV3	45163	55718	5.42%	0.639%
15	9.722	1296	1298	1301	rVB	51215	44754	4.35%	0.514%
16	9.816	1311	1314	1317	rVB	404690	327888	31.90%	3.763%
17	10.222	1380	1383	1385	rBV2	64592	59402	5.78%	0.682%
18	10.616	1447	1450	1454	rBV	567551	524368	51.01%	6.018%
19	11.316	1566	1569	1572	rBV	402636	352831	34.32%	4.049%
20	11.686	1629	1632	1635	rVB	997127	788149	76.67%	9.045%
21	11.851	1658	1660	1664	rVB2	177688	155593	15.14%	1.786%
22	12.386	1748	1751	1754	rBV	966925	742591	72.24%	8.522%
23	12.910	1837	1840	1843	rBV	1185285	1028020	100.00%	11.798%
24	13.974	2018	2021	2024	rVB	399756	334431	32.53%	3.838%
25	15.462	2269	2274	2279	rBV	307200	395964	38.52%	4.544%

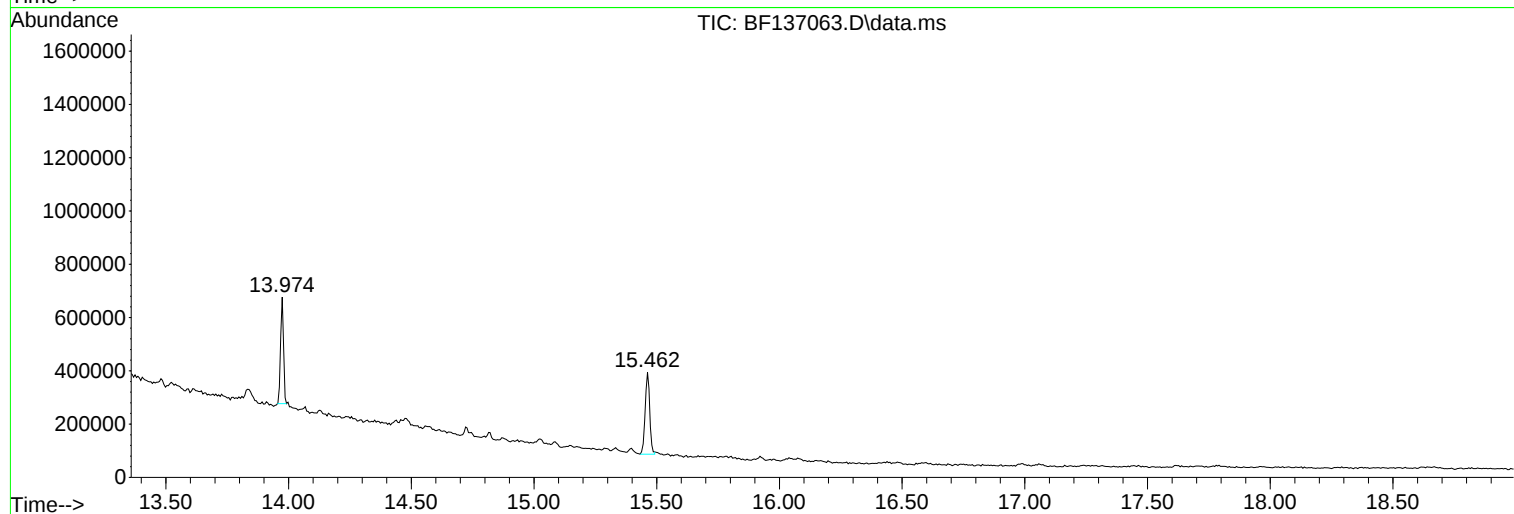
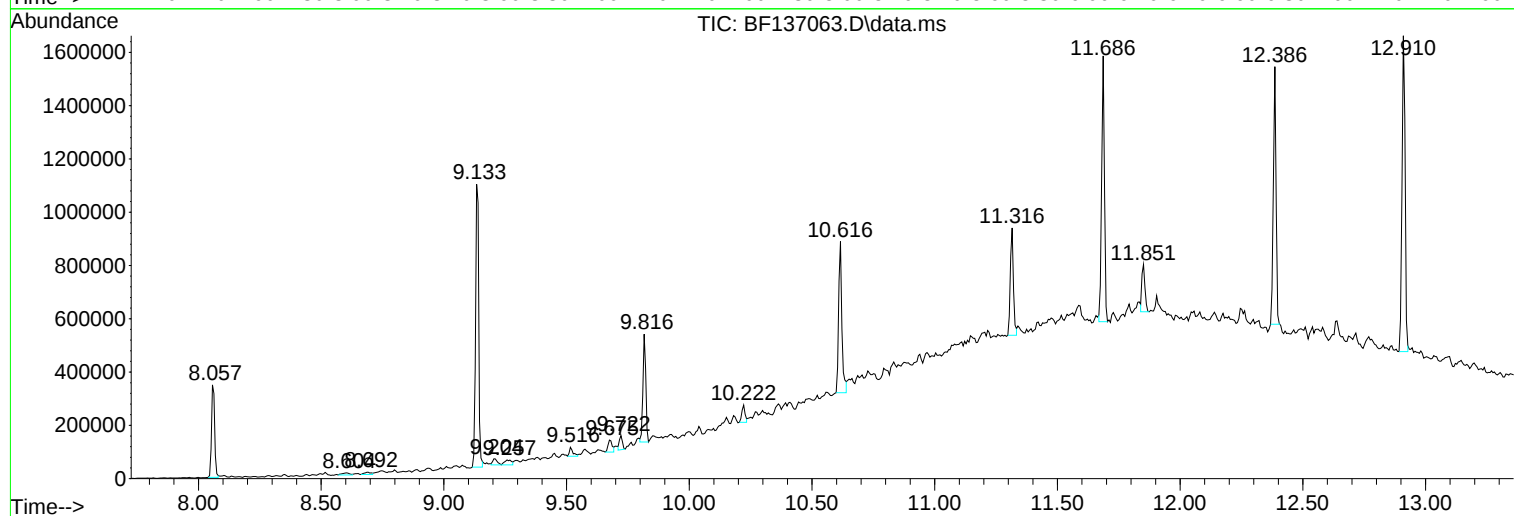
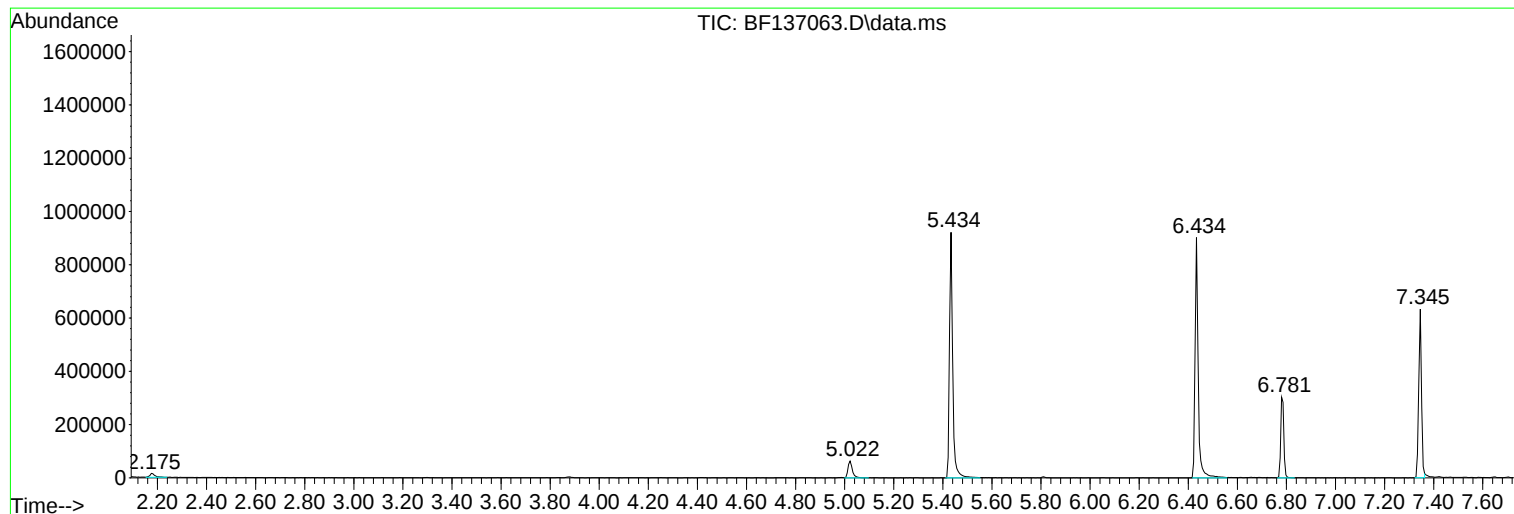
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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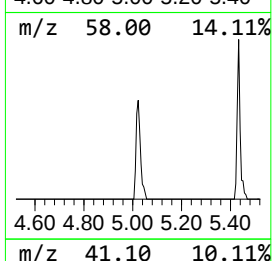
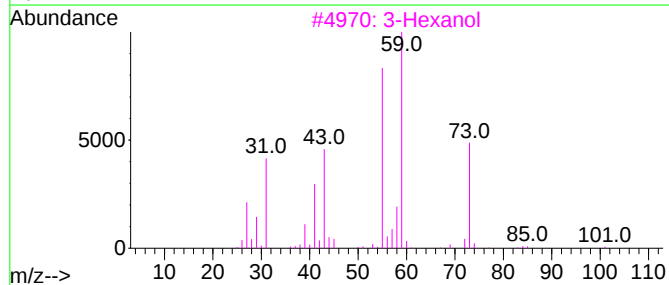
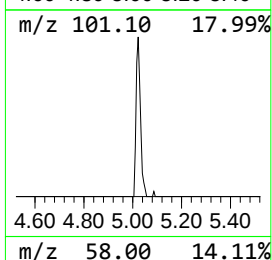
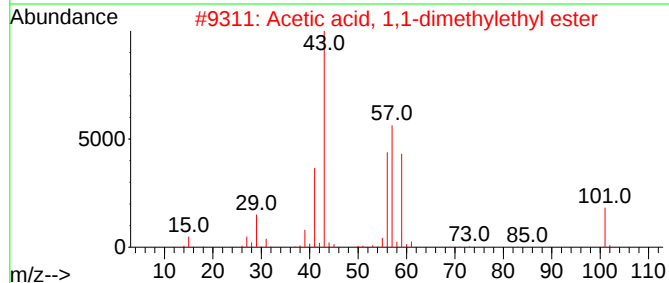
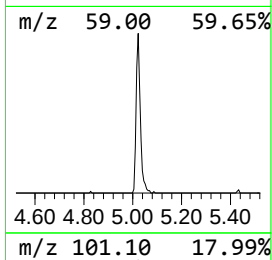
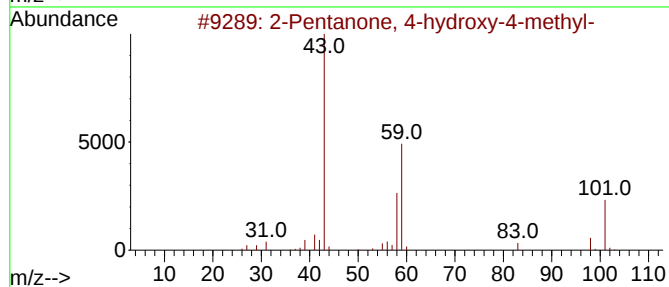
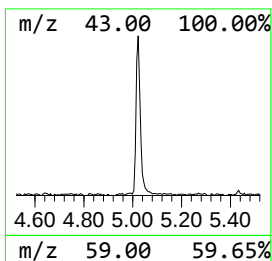
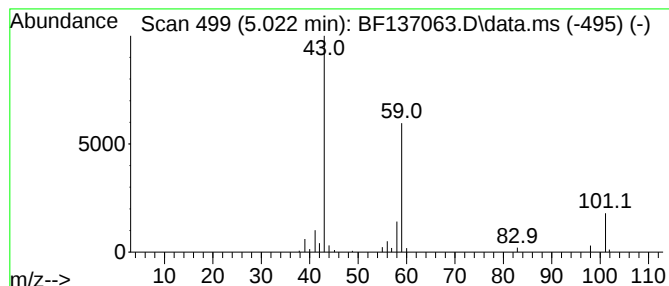
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.84 ng	77554	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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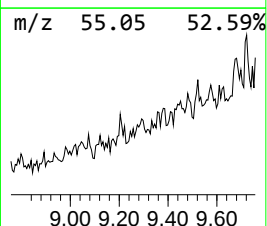
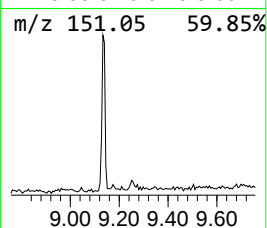
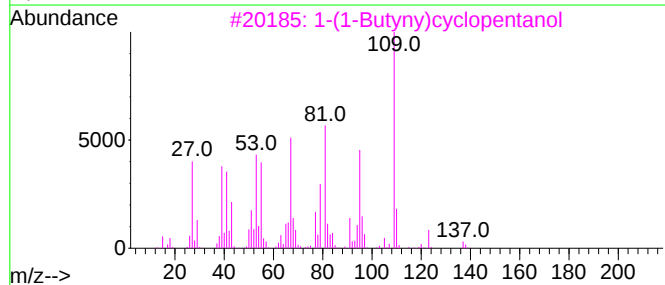
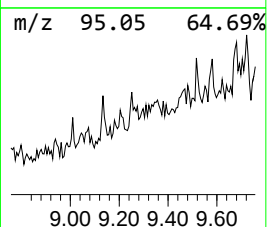
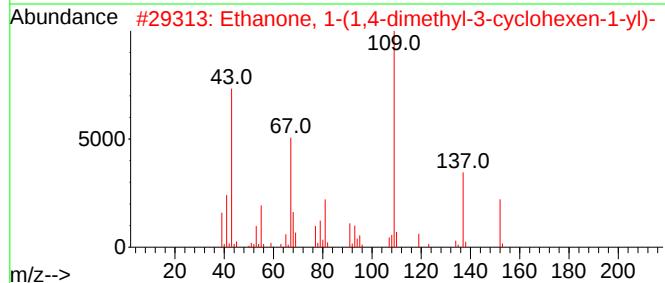
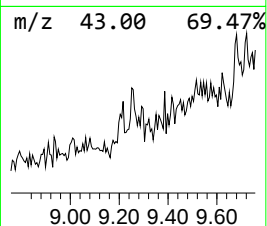
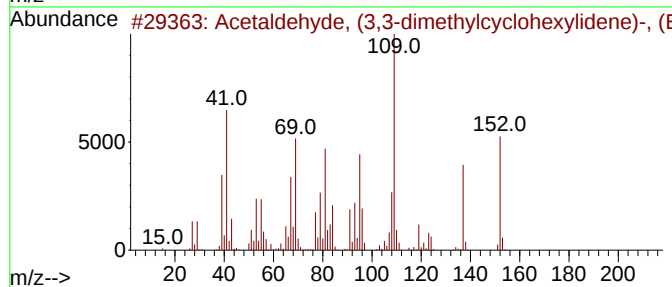
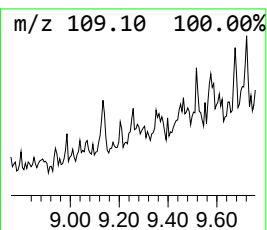
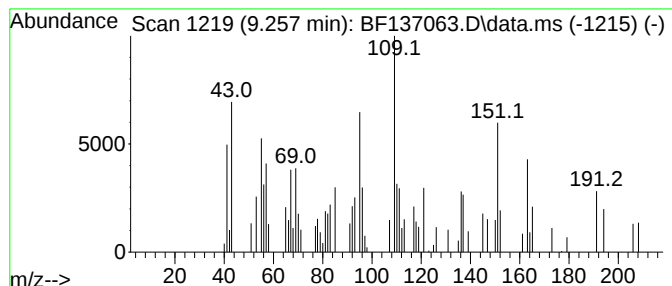
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Peak Number 2 unknown9.257 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	2.23 ng	36594	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	41
2		Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	30
3		1-(1-Butyny)cyclopentanol	138	C9H14O	1000342-86-5	27
4		3,3-Dimethyl-5-methylenehept-6-e...	152	C10H16O	1010424-30-5	22
5		2-Cyclohexen-1-one, 3,5,5-trimet...	208	C13H20O2	074233-41-3	22



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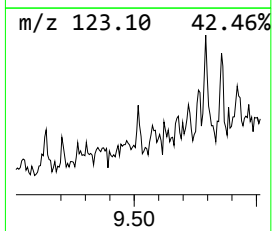
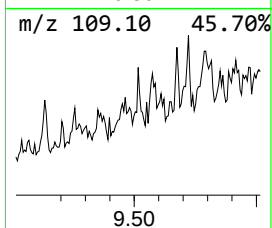
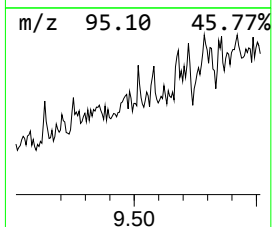
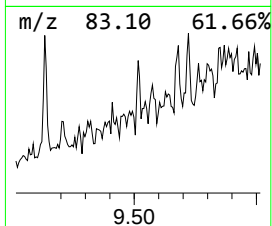
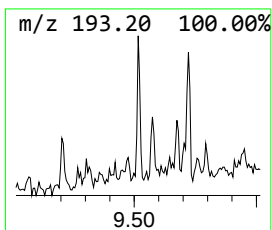
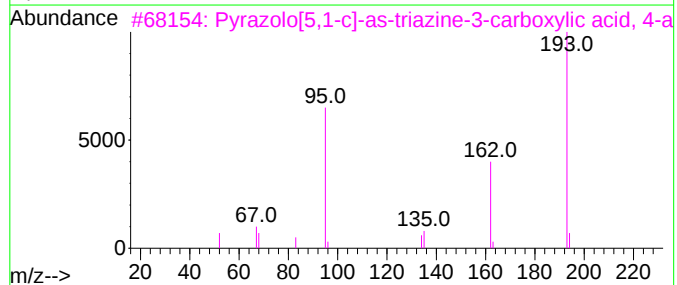
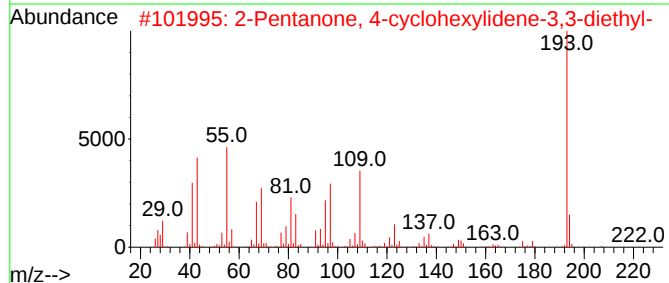
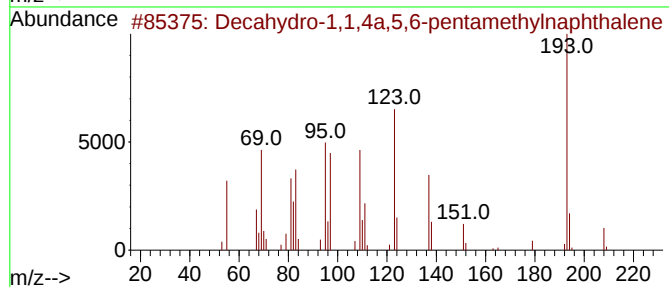
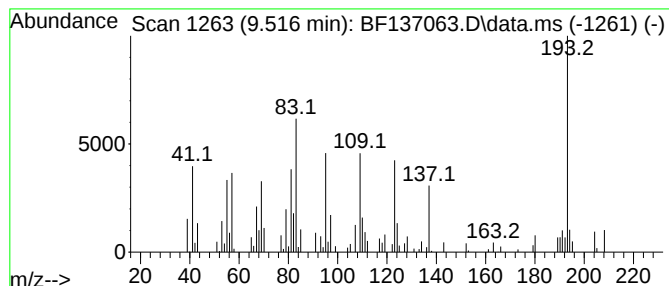
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Peak Number 3 unknown9.516 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.516	2.13 ng	34995	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	47		
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37		
3	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35		
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	22		
5	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	16		



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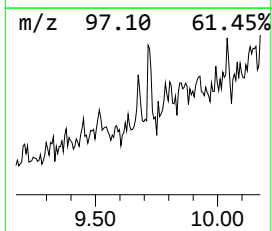
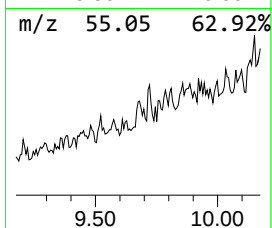
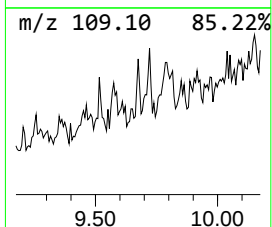
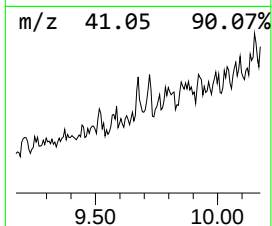
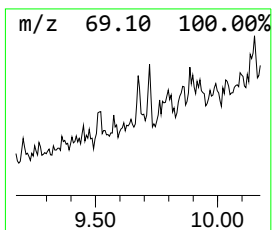
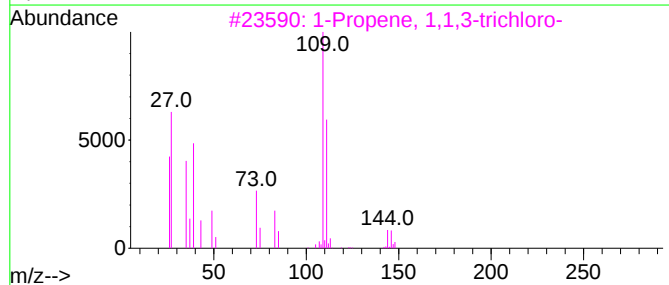
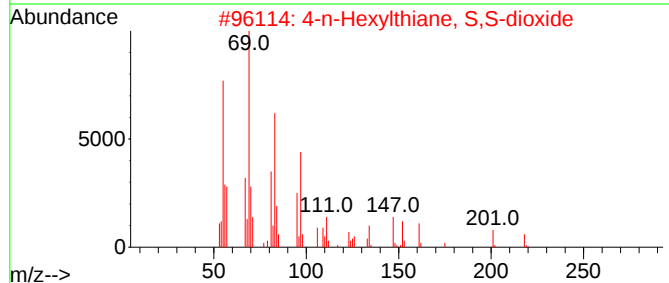
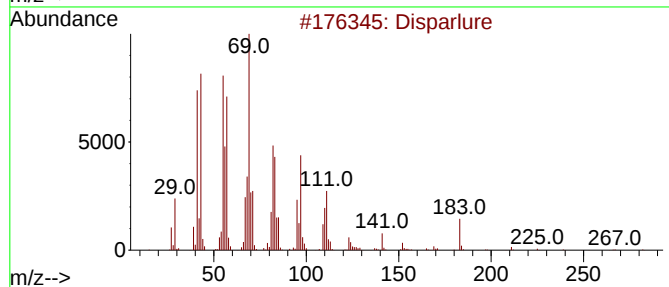
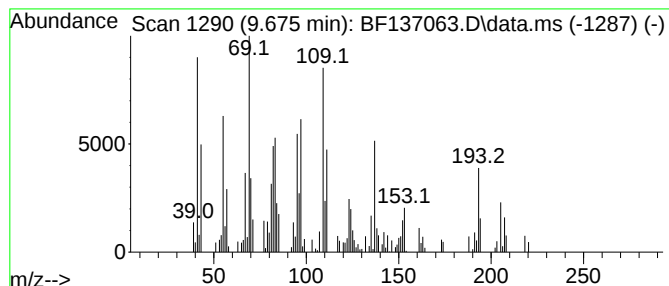
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Peak Number 4 unknown9.675 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.675	3.40 ng	55718	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disparlure	282	C19H38O	029804-22-6	27
2			4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	20
3			1-Propene, 1,1,3-trichloro-	144	C3H3Cl3	002567-14-8	18
4			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	18
5			1,3,3,5,5-Pentamethylcyclohexanol	170	C11H22O	038490-33-4	14



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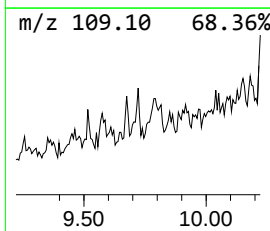
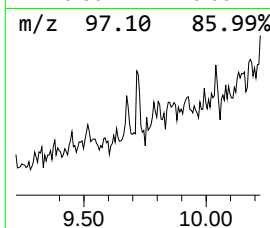
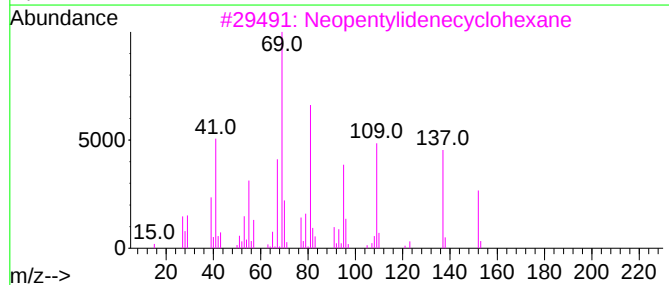
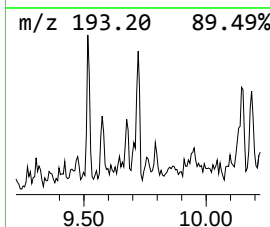
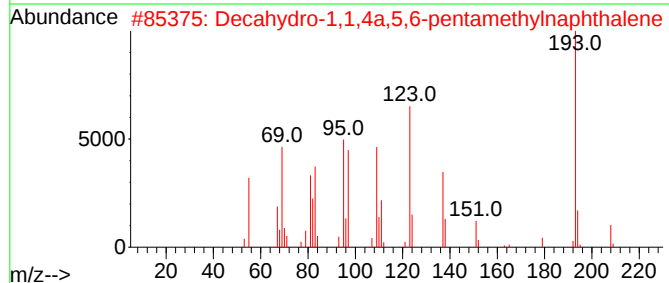
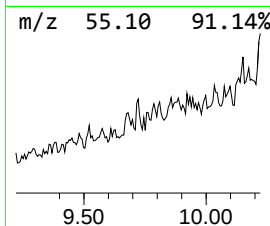
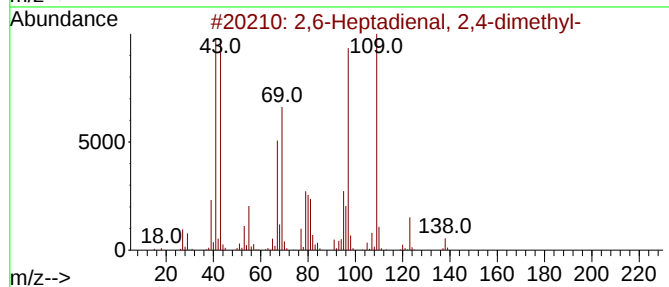
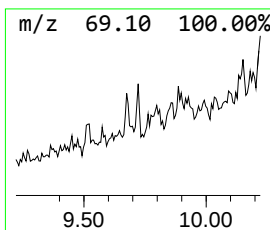
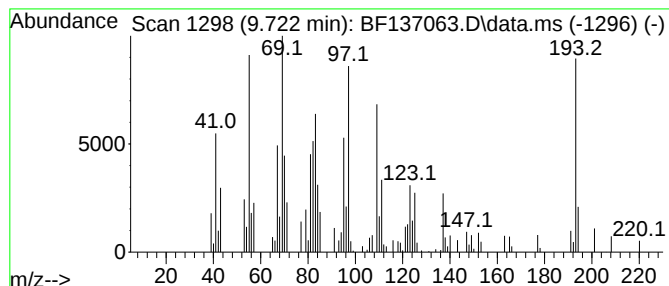
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Peak Number 5 unknown9.722 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	2.73 ng	44754	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
2			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
3			Neopentylidenecyclohexane	152	C11H20	039546-80-0	25
4			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	18
5			Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	14



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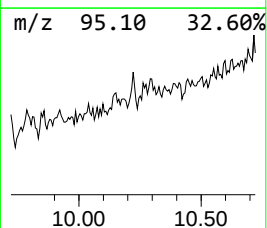
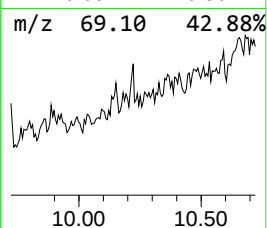
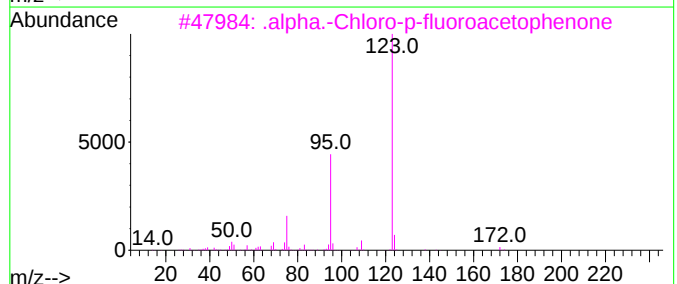
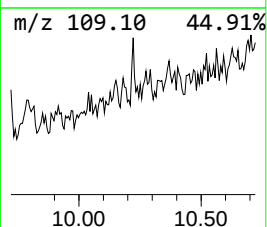
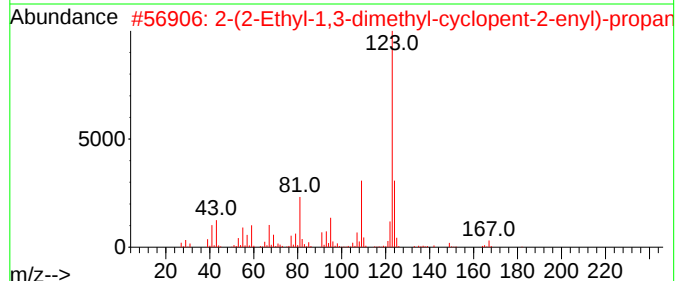
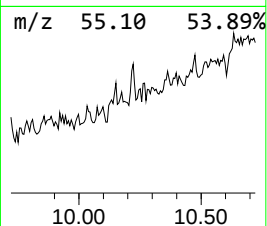
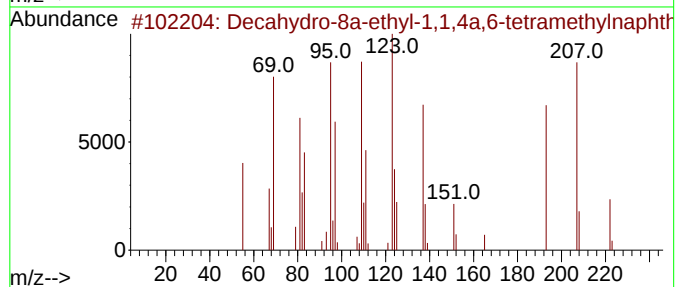
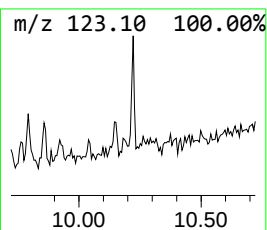
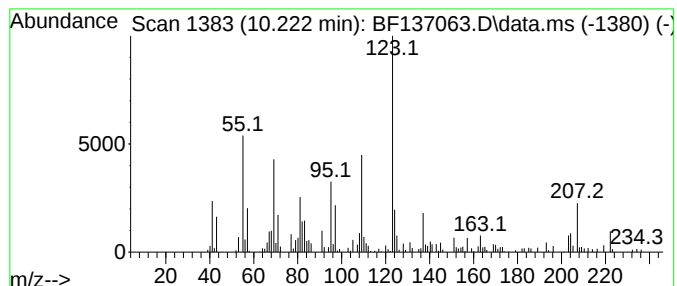
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.222	3.62 ng	59402	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	70
2			2-(2-Ethyl-1,3-dimethyl-cyclopent...	182	C12H22O	1000186-82-4	50
3			.alpha.-Chloro-p-fluoroacetophenone	172	C8H6ClFO	000456-04-2	38
4			Benzamide, 3-fluoro-N-(2-phenyle...	313	C20H24FNO	1000451-30-5	38
5			2-Fluoro-N-(1,3-thiazol-2-yl)ben...	222	C10H7FN2OS	000319-38-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137063.D
Acq On : 15 Jan 2024 15:11
Operator : CG\JU
Sample : P1132-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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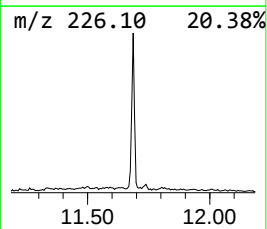
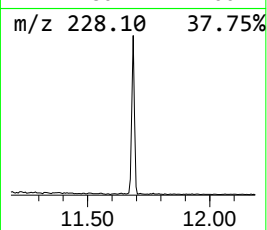
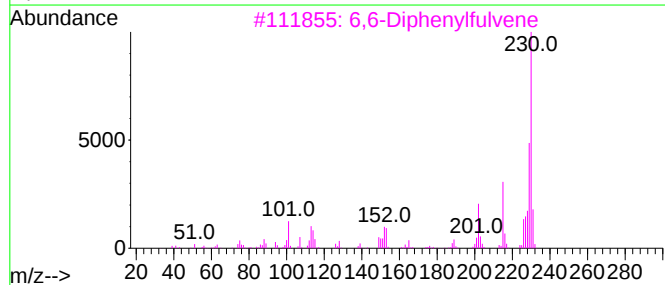
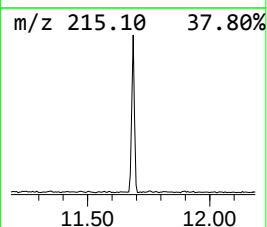
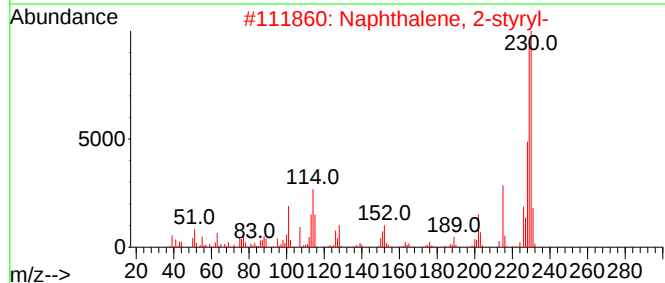
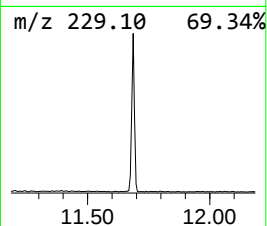
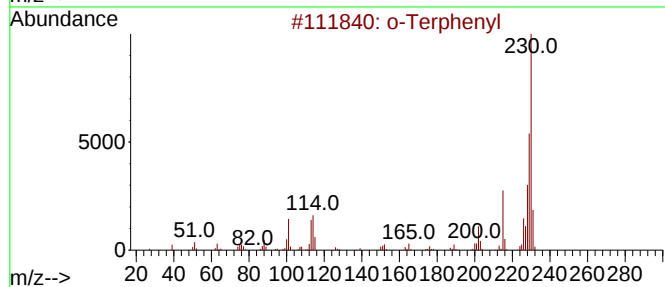
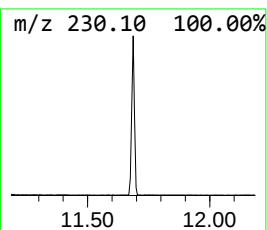
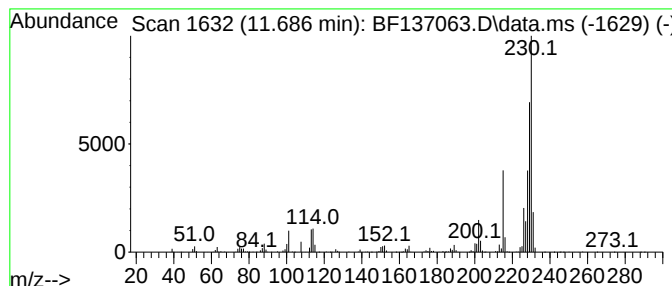
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 o-Terphenyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.686	44.68 ng	788149	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Terphenyl	230	C18H14	000084-15-1	98
2			Naphthalene, 2-styryl-	230	C18H14	002039-70-5	93
3			6,6-Diphenylfulvene	230	C18H14	002175-90-8	93
4			Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	86
5			Naphthacene, 5,12-dihydro-	230	C18H14	000959-02-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137063.D
Acq On : 15 Jan 2024 15:11
Operator : CG\JU
Sample : P1132-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200010

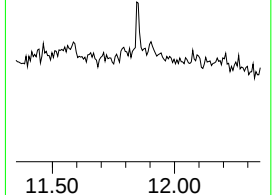
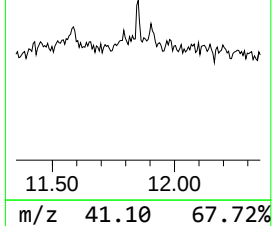
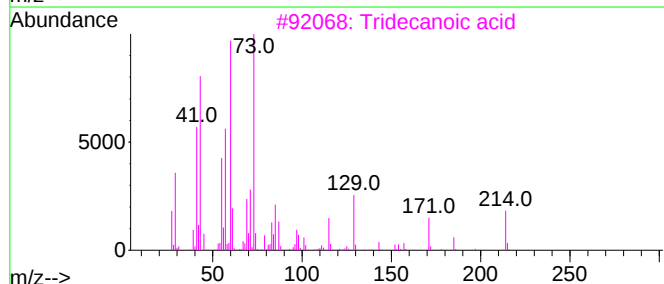
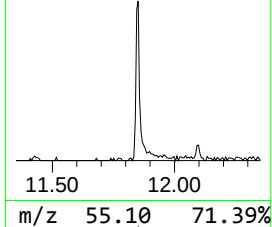
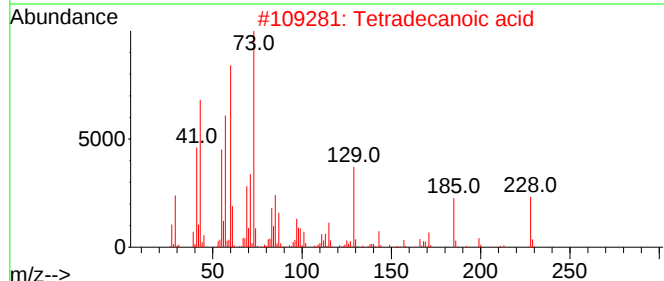
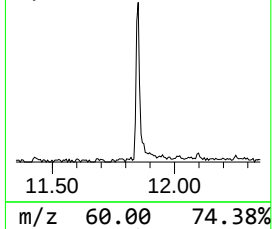
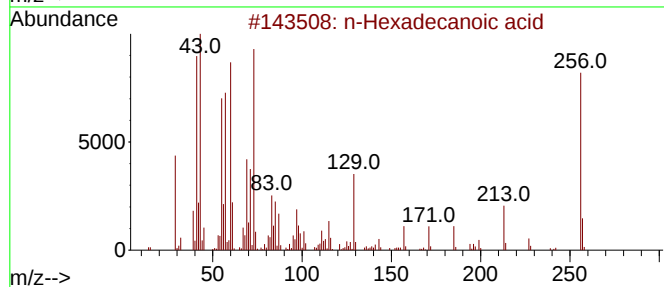
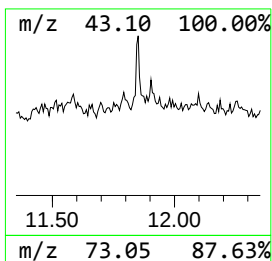
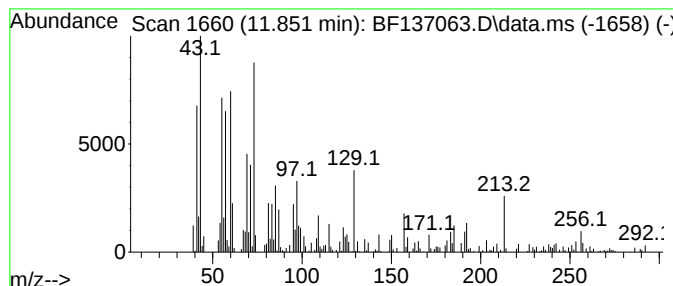
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	8.82 ng	155593	Phenanthrene-d10	11.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3		Tridecanoic acid	214	C13H26O2	000638-53-9	62
4		Octadecanoic acid	284	C18H36O2	000057-11-4	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137063.D
Acq On : 15 Jan 2024 15:11
Operator : CG\JU
Sample : P1132-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

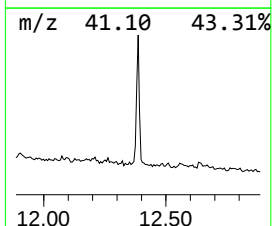
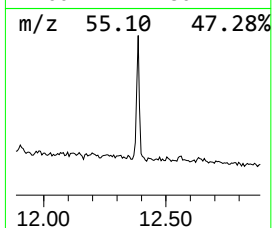
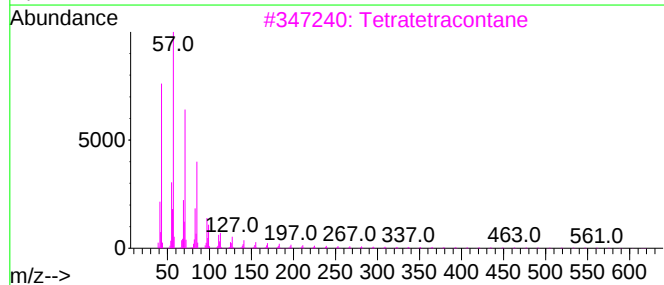
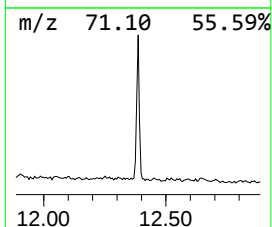
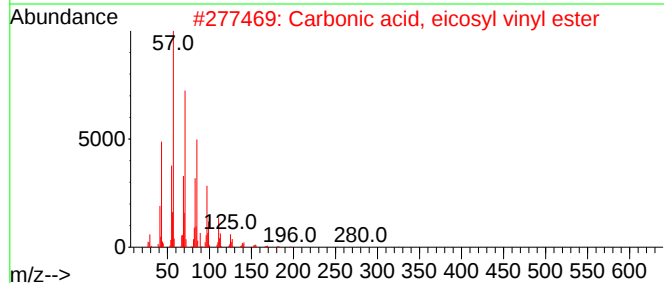
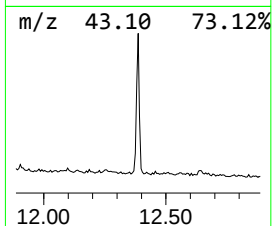
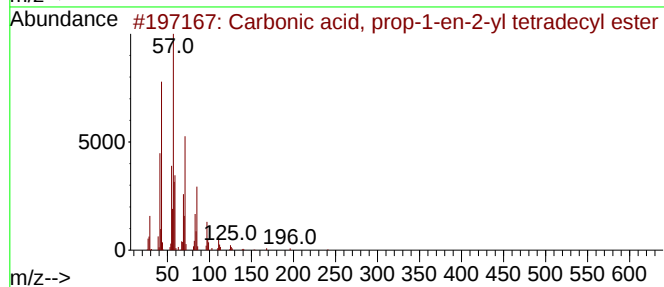
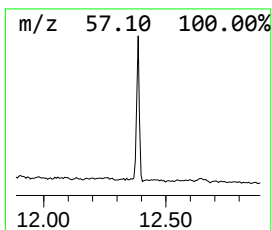
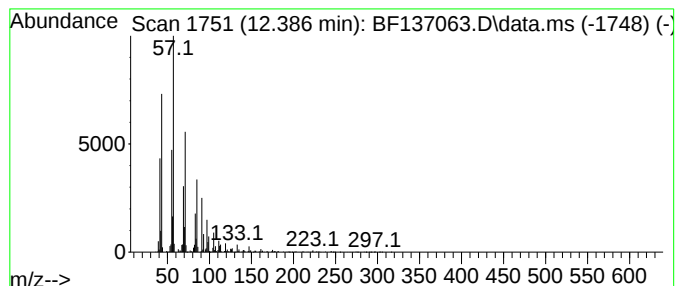
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Carbonic acid, prop-1-en-2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.386	42.09 ng	742591	Phenanthrene-d10		11.316	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Carbonic acid, prop-1-en-2-yl te...		298	C18H34O3	1000382-90-9	72
2	Carbonic acid, eicosyl vinyl ester		368	C23H44O3	1000382-54-3	72
3	Tetratetracontane		619	C44H90	007098-22-8	64
4	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	64
5	Hexadecane, 1-chloro-		260	C16H33Cl	004860-03-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137063.D
Acq On : 15 Jan 2024 15:11
Operator : CG\JU
Sample : P1132-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200010

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.022	5.8	ng	77554	1	6.781	265488	20.0
unknown9.257	9.257	2.2	ng	36594	3	9.816	327888	20.0
unknown9.516	9.516	2.1	ng	34995	3	9.816	327888	20.0
unknown9.675	9.675	3.4	ng	55718	3	9.816	327888	20.0
unknown9.722	9.722	2.7	ng	44754	3	9.816	327888	20.0
Decahydro-8a-et...	10.222	3.6	ng	59402	3	9.816	327888	20.0
o-Terphenyl	11.686	44.7	ng	788149	4	11.316	352831	20.0
n-Hexadecanoic ...	11.851	8.8	ng	155593	4	11.316	352831	20.0
Carbonic acid, ...	12.386	42.1	ng	742591	4	11.316	352831	20.0