

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
 Data File : BF137561.D
 Acq On : 11 Mar 2024 17:47
 Operator : CG\JU
 Sample : P1720-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT3471

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	24	33	42	rVB	1043508	1447030	27.42%	3.422%
2	5.569	588	592	615	rBV	4827944	4863368	92.17%	11.500%
3	6.192	695	698	701	rBV	267994	214518	4.07%	0.507%
4	6.545	753	758	765	rBV	4576097	4974505	94.27%	11.763%
5	6.604	765	768	774	rVB	216567	216647	4.11%	0.512%
6	6.898	815	818	829	rBV	1523556	1364205	25.85%	3.226%
7	7.457	909	913	931	rBV	3213776	3124572	59.22%	7.389%
8	8.104	1019	1023	1026	rBV	952522	789405	14.96%	1.867%
9	8.169	1030	1034	1053	rVB	2066607	1902451	36.05%	4.499%
10	9.251	1213	1218	1221	rBV	5804992	5276630	100.00%	12.477%
11	9.557	1267	1270	1272	rBV3	155190	147520	2.80%	0.349%
12	9.839	1315	1318	1321	rVB2	125331	128736	2.44%	0.304%
13	9.880	1321	1325	1326	rBV3	89634	123713	2.34%	0.293%
14	9.928	1326	1333	1337	rBV	2648204	2385672	45.21%	5.641%
15	10.192	1376	1378	1380	rBV2	128615	104197	1.97%	0.246%
16	10.339	1400	1403	1405	rBV2	152554	173846	3.29%	0.411%
17	10.592	1444	1446	1452	rVB	326565	359661	6.82%	0.850%
18	10.722	1464	1468	1472	rBV	2450437	2630015	49.84%	6.219%
19	10.804	1480	1482	1487	rBV5	210796	278953	5.29%	0.660%
20	10.863	1489	1492	1495	rVB	757886	723886	13.72%	1.712%
21	11.057	1523	1525	1527	rBV	252304	209110	3.96%	0.494%
22	11.333	1568	1572	1575	rVB	1203530	1226612	23.25%	2.901%
23	11.427	1585	1588	1593	rBV	1808610	1816802	34.43%	4.296%
24	12.492	1767	1769	1772	rVB	391709	324691	6.15%	0.768%
25	13.033	1857	1861	1864	rBV	3738618	3542164	67.13%	8.376%
26	13.951	2014	2017	2029	rVB	338799	498498	9.45%	1.179%
27	14.092	2037	2041	2052	rVB	1236977	1447092	27.42%	3.422%
28	14.580	2121	2124	2127	rBV	240777	222027	4.21%	0.525%
29	15.174	2223	2225	2235	rVB	56394	122357	2.32%	0.289%
30	15.292	2241	2245	2249	rVB2	104992	131696	2.50%	0.311%
31	15.574	2290	2293	2299	rVB2	44961	69852	1.32%	0.165%
32	15.639	2299	2304	2314	rBV	890317	1269278	24.05%	3.001%
33	16.215	2398	2402	2409	rVB2	65075	114981	2.18%	0.272%
34	17.498	2615	2620	2626	rVB2	32293	64788	1.23%	0.153%

Sum of corrected areas: 42289478

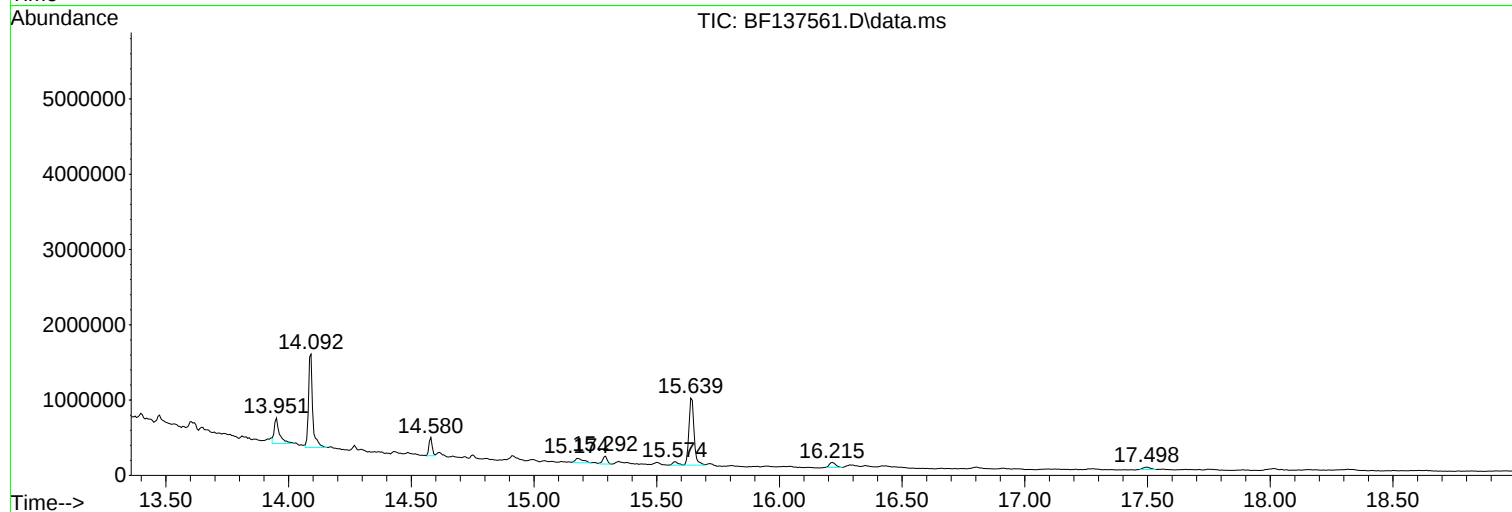
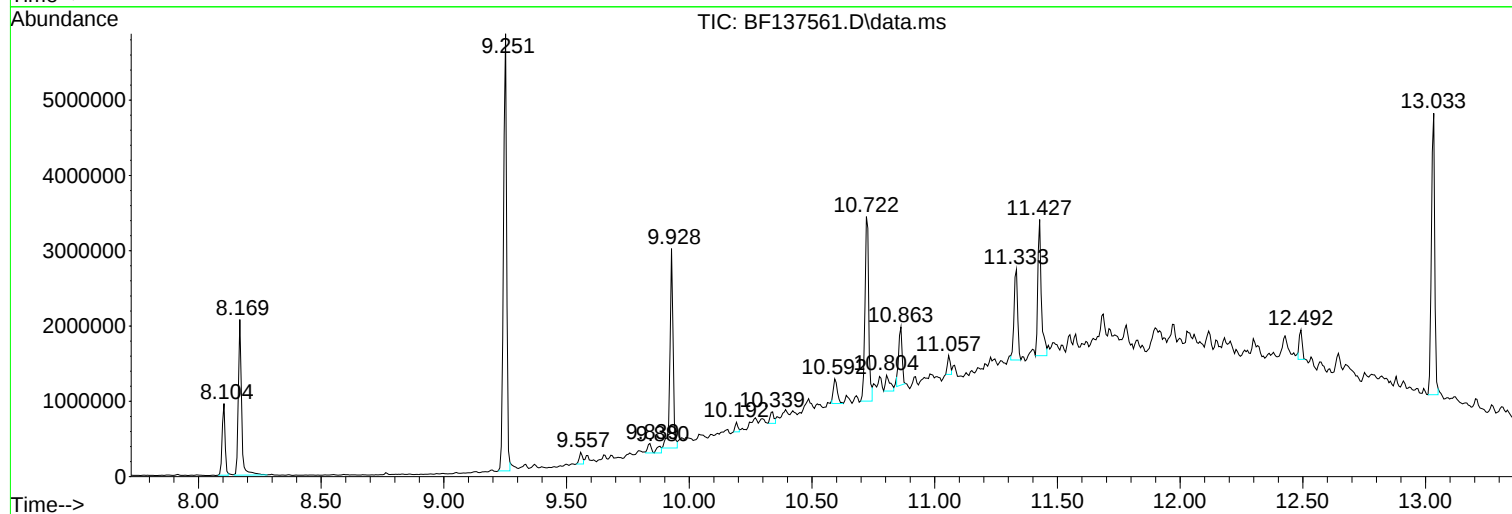
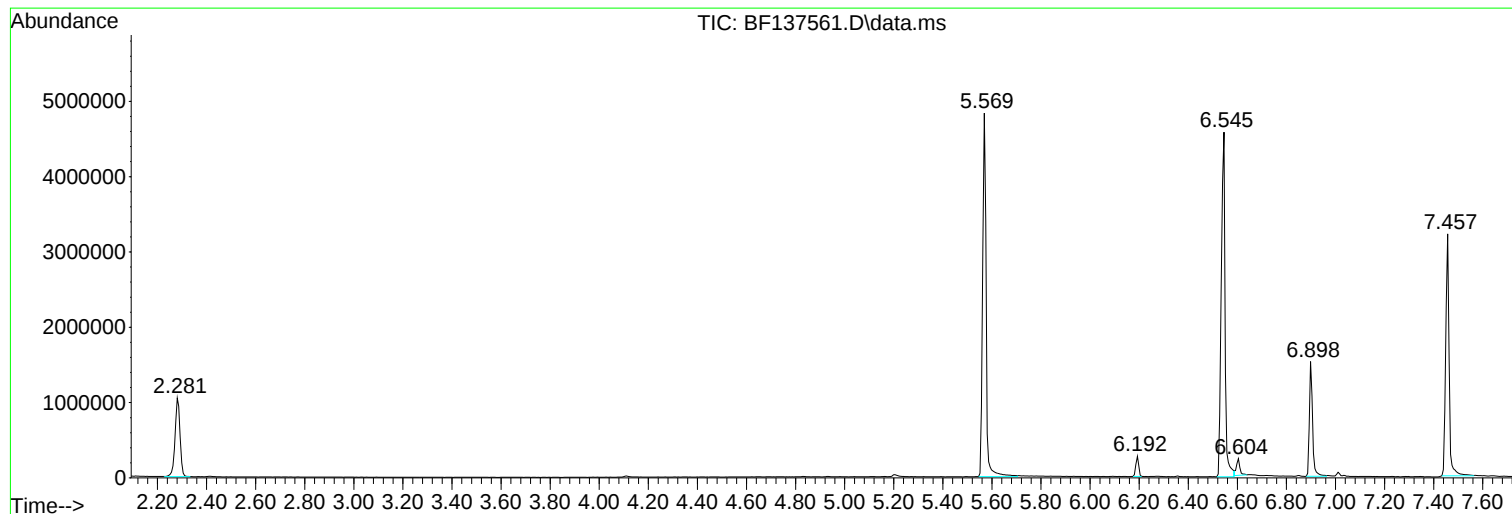
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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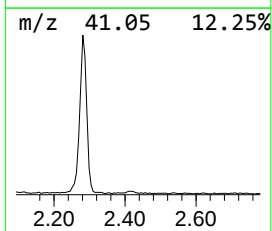
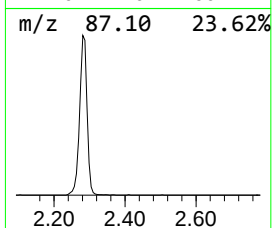
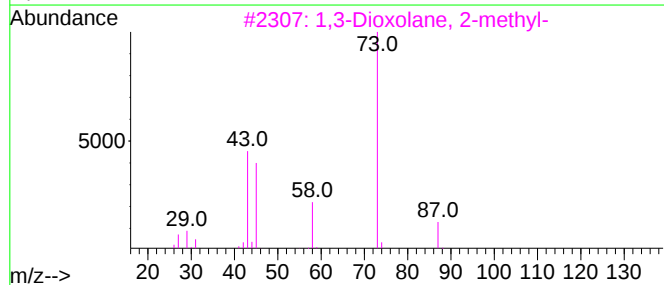
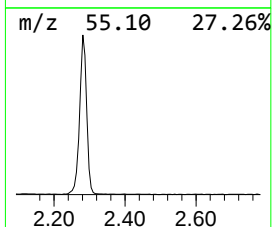
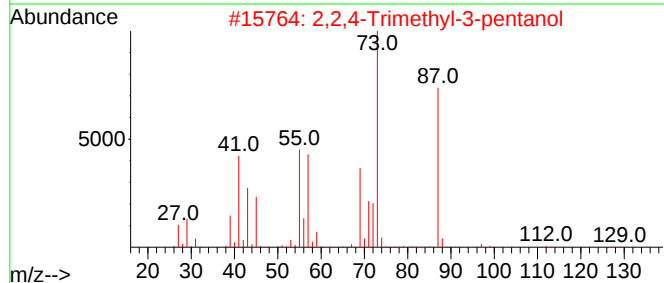
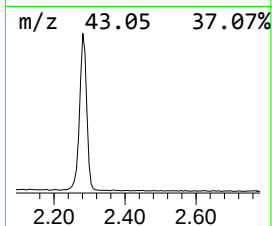
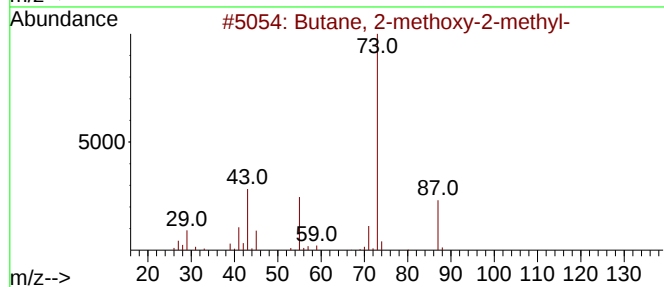
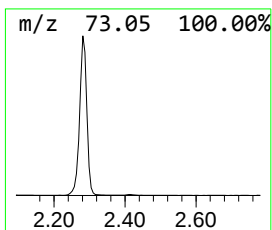
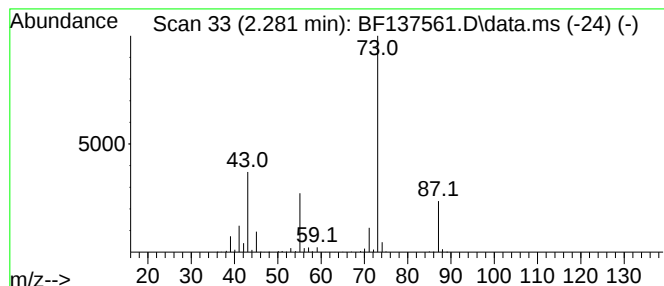
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.281	21.21 ng	1447030	1,4-Dichlorobenzene-d4	6.898

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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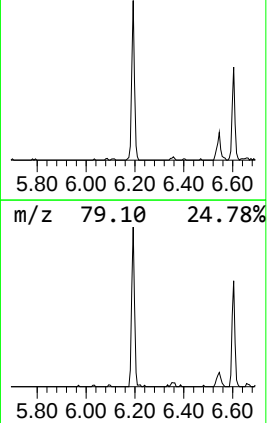
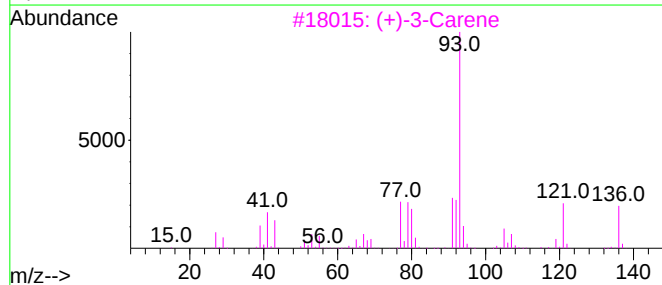
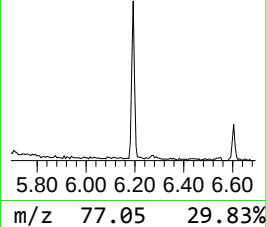
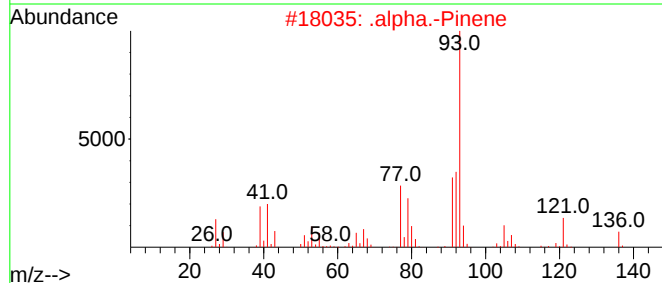
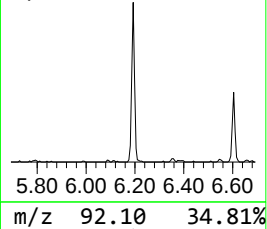
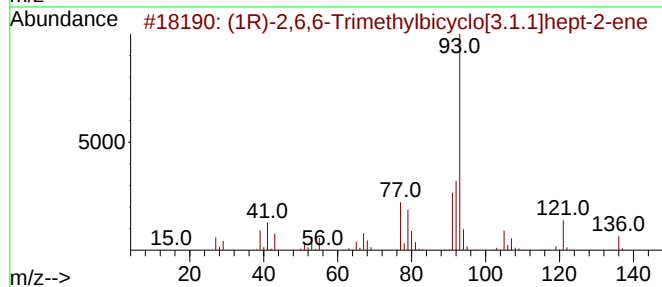
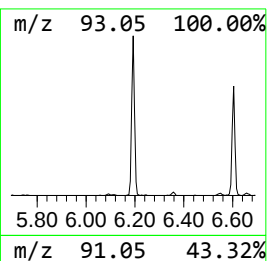
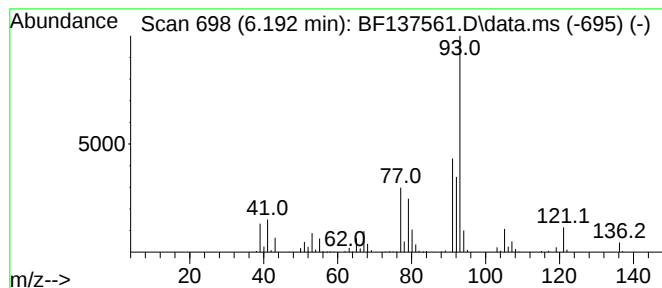
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.192	3.14 ng	214518	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	97		
2	.alpha.-Pinene	136	C10H16	000080-56-8	95		
3	(+)-3-Carene	136	C10H16	000498-15-7	91		
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91		
5	Tricyclo[2.2.1.0(2,6)]heptane, 1,1,2-trimethyl-	136	C10H16	000508-32-7	91		



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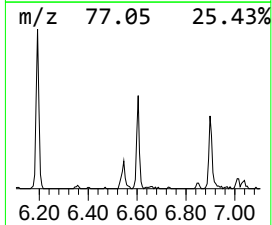
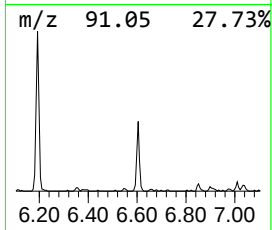
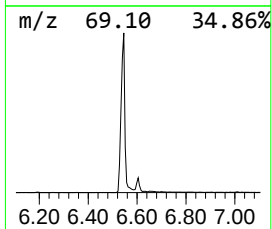
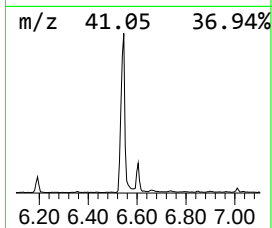
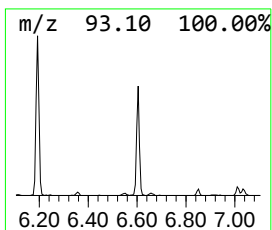
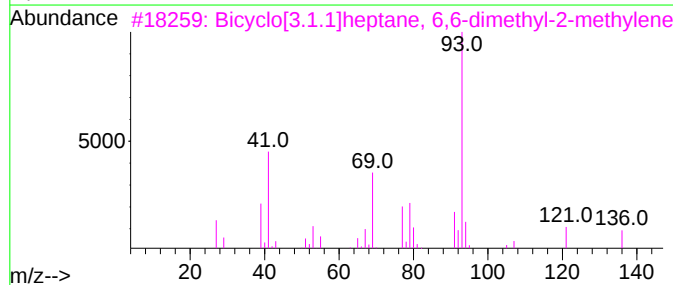
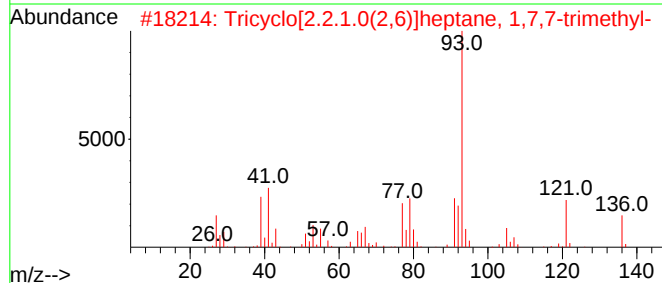
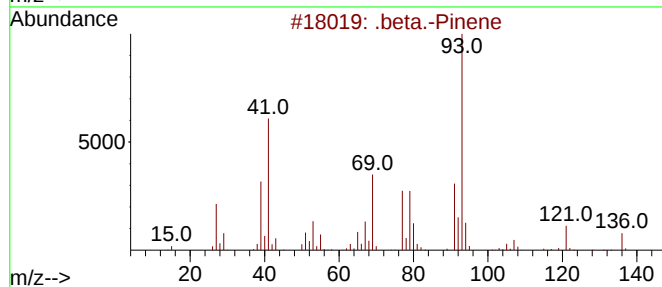
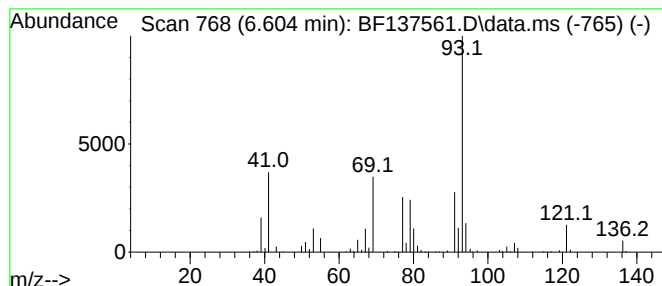
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 .beta.-Pinene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	3.18 ng	216647	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Pinene	136	C10H16	000127-91-3	96	
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91		
3	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91		
4	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	91		
5	.alpha.-Pinene	136	C10H16	000080-56-8	90		



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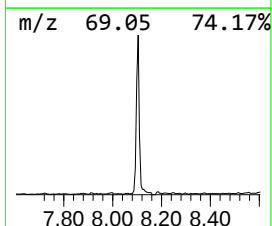
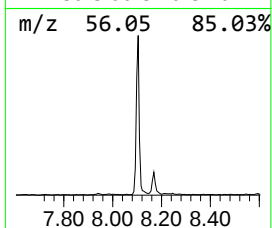
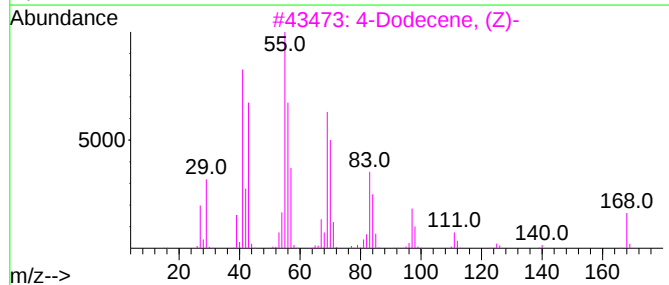
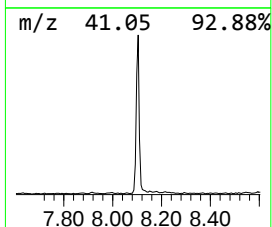
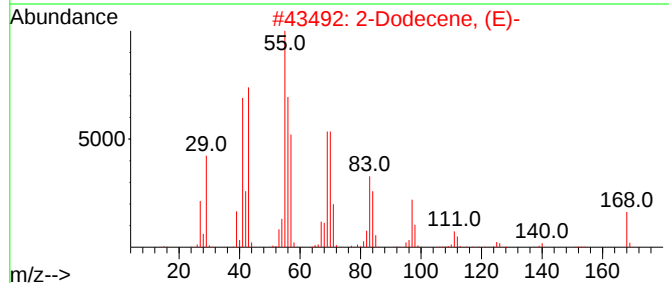
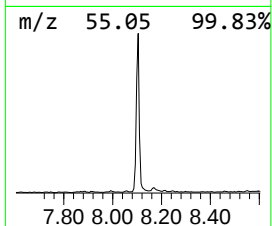
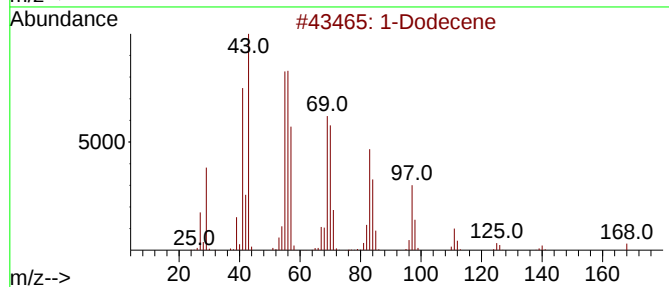
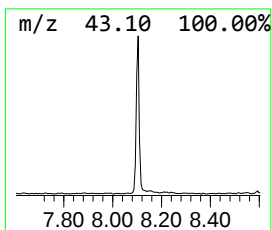
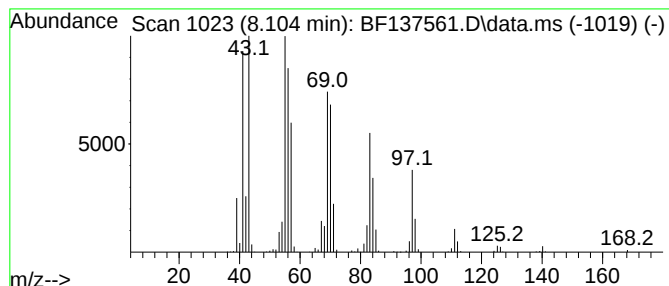
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Peak Number 4 1-Dodecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	8.30 ng	789405	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecene			168	C12H24	000112-41-4	96
2	2-Dodecene, (E)-			168	C12H24	007206-13-5	94
3	4-Dodecene, (Z)-			168	C12H24	007206-27-1	91
4	1-Decene			140	C10H20	000872-05-9	90
5	4-Dodecene, (E)-			168	C12H24	007206-15-7	90



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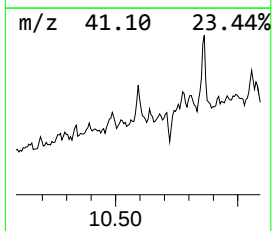
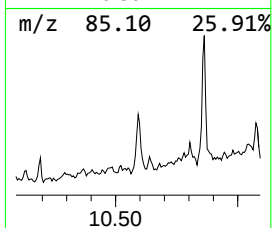
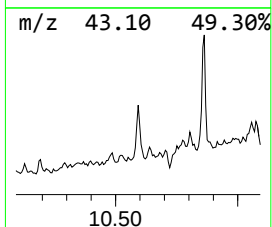
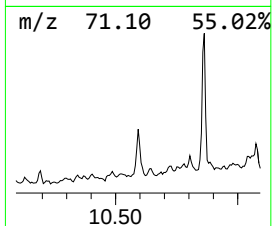
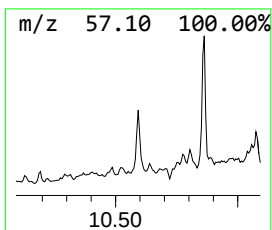
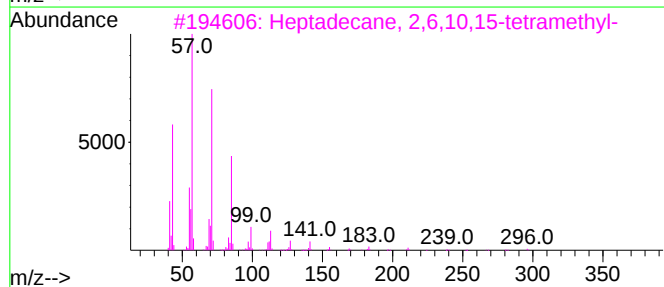
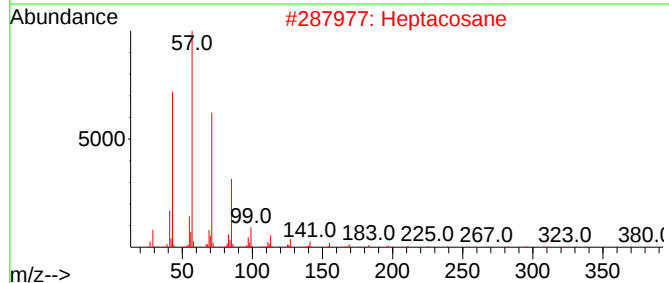
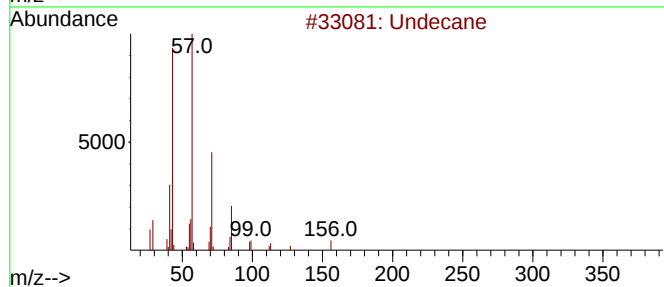
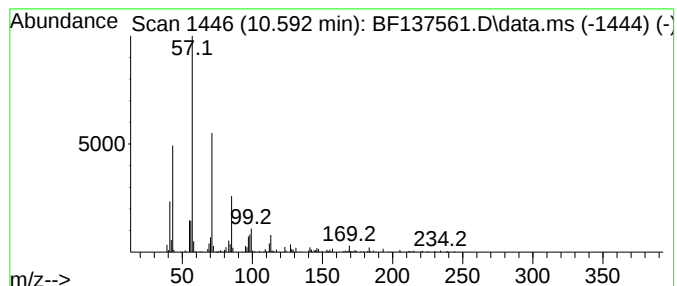
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Peak Number 5 Undecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	3.02 ng	359661	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	76
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



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ClientSampleId :
RT3471

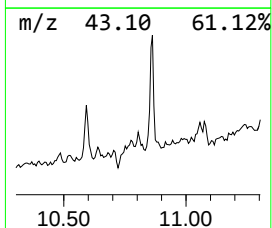
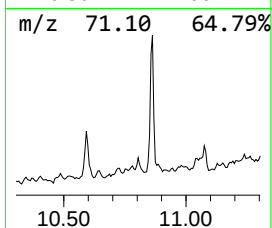
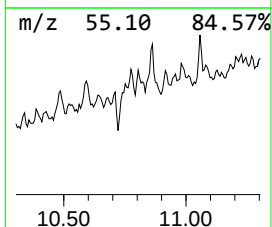
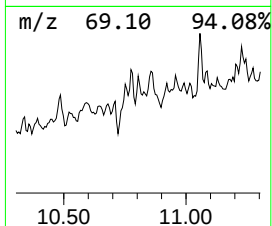
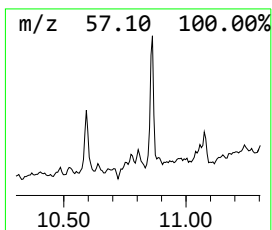
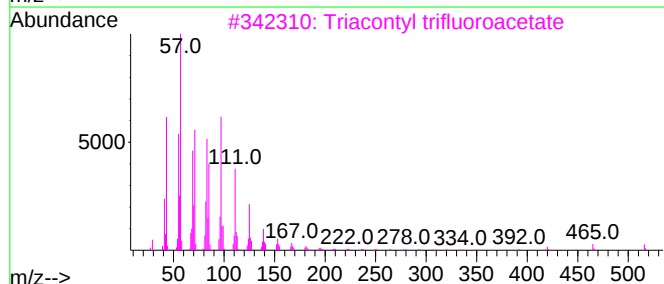
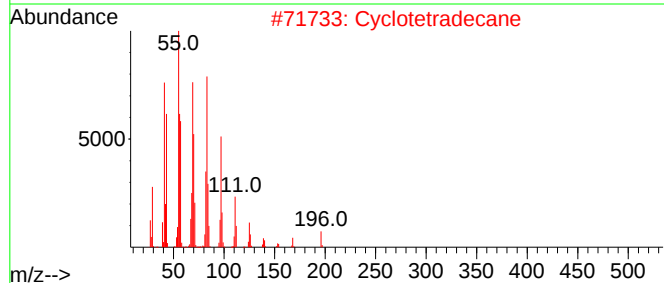
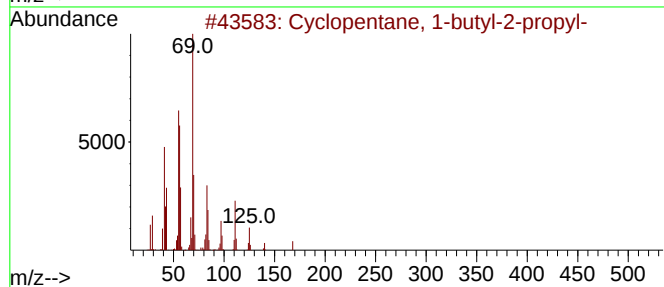
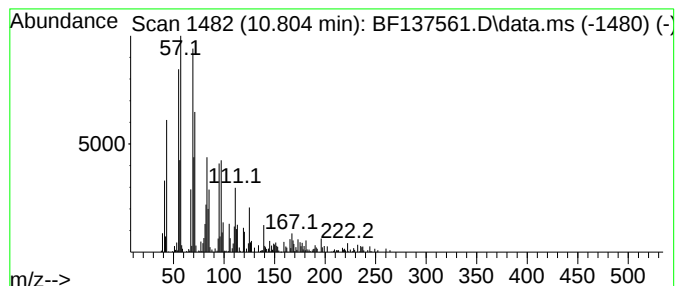
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentane, 1-butyl-2-pro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	3.07 ng	278953	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	64
2			Cyclotetradecane	196	C14H28	000295-17-0	64
3			Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	49
4			Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	49
5			Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137561.D
Acq On : 11 Mar 2024 17:47
Operator : CG\JU
Sample : P1720-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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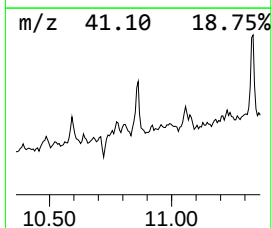
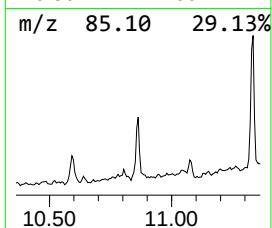
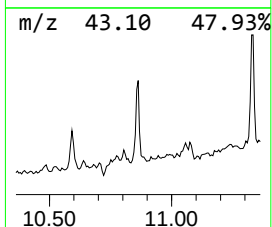
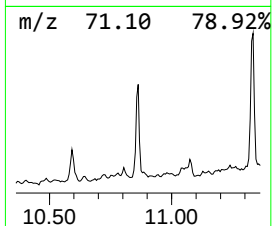
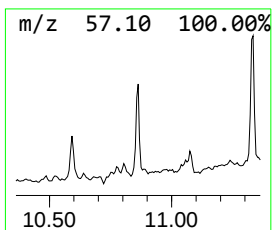
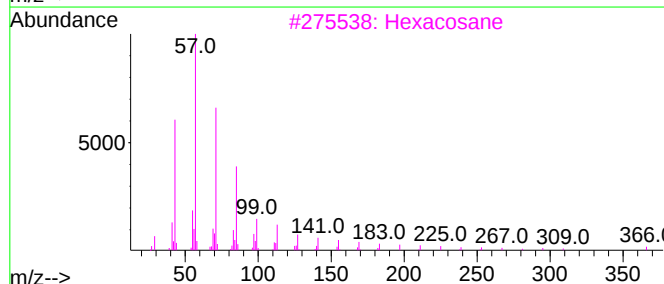
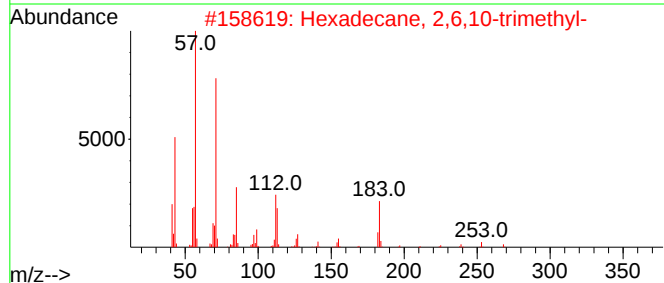
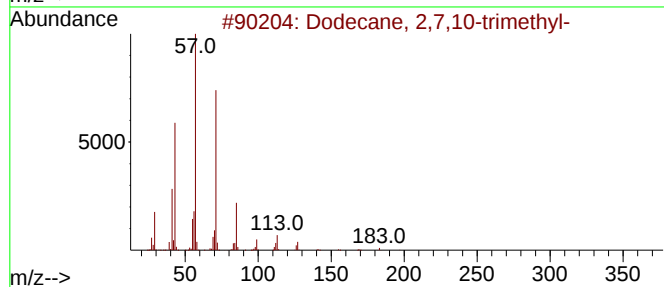
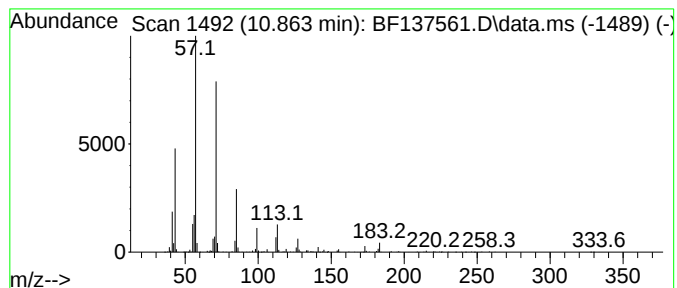
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Dodecane, 2,7,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.863	7.97 ng	723886	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2			Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	83
3			Hexacosane	366	C26H54	000630-01-3	78
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
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Instrument :
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ClientSampleId :
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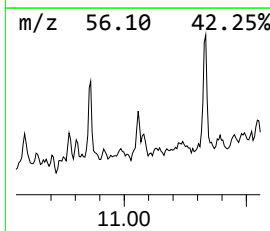
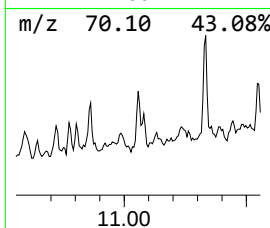
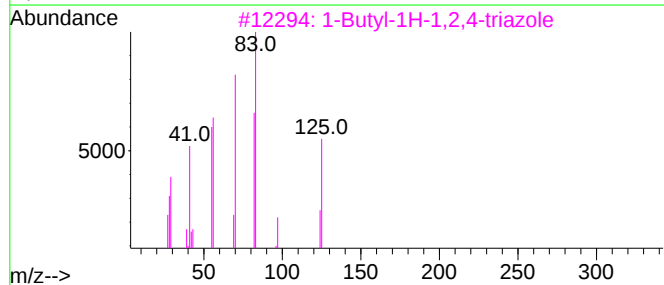
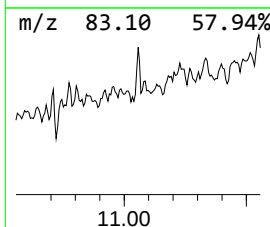
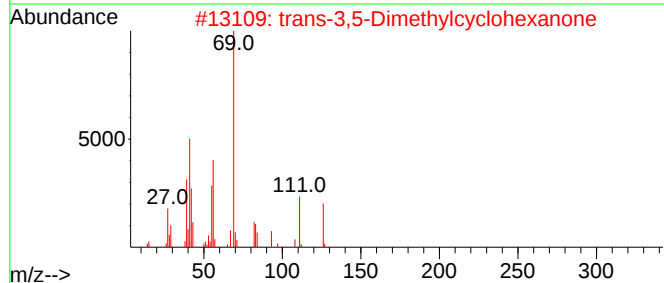
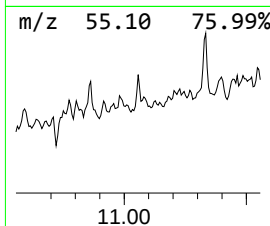
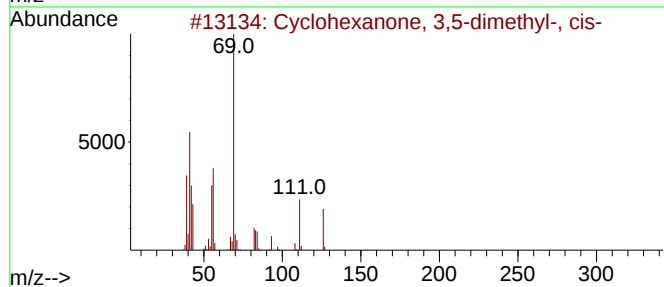
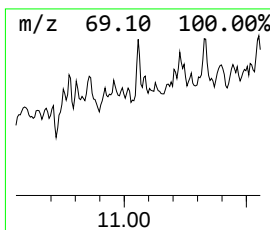
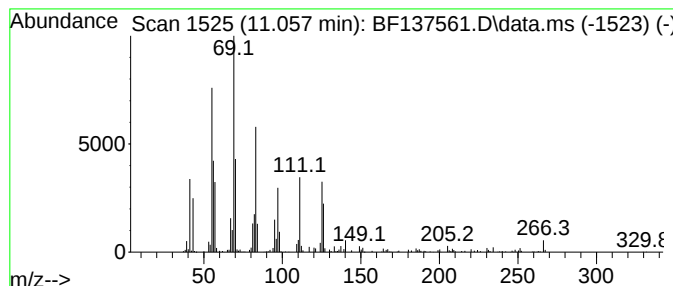
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.057 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.057	2.30 ng	209110	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,5-dimethyl-, cis-	126	C8H14O	007214-52-0	49
2			trans-3,5-Dimethylcyclohexanone	126	C8H14O	007214-49-5	49
3			1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	46
4			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	43
5			Cyclohexanone, 3,5-dimethyl-	126	C8H14O	002320-30-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
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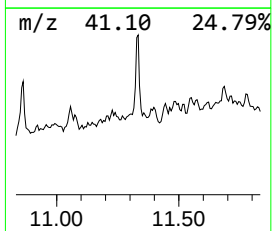
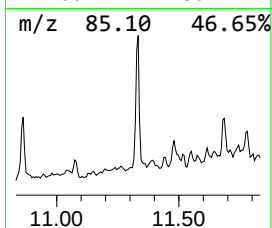
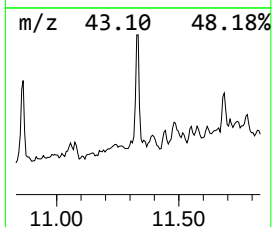
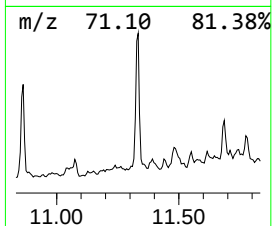
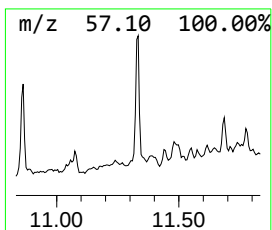
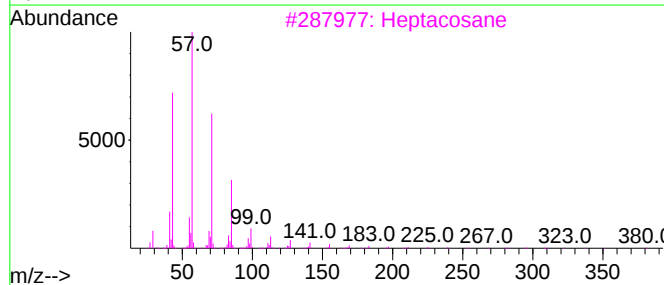
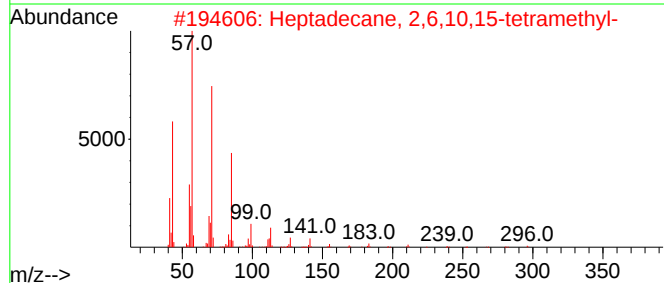
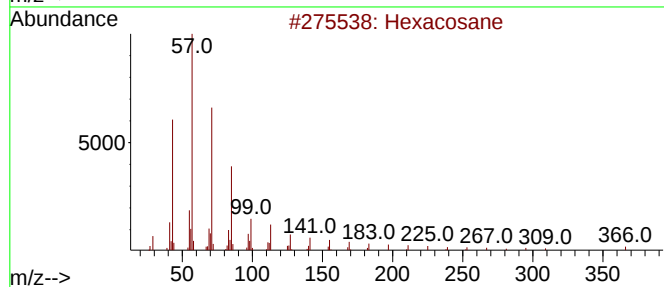
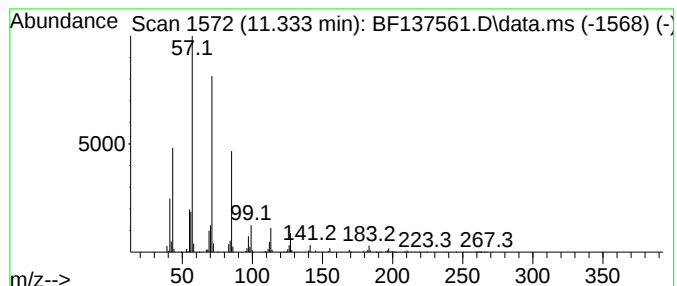
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.333	13.50 ng	1226610	Phenanthrene-d10	11.427	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	83
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
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Instrument :
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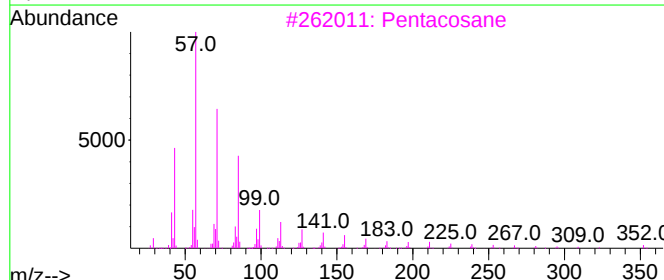
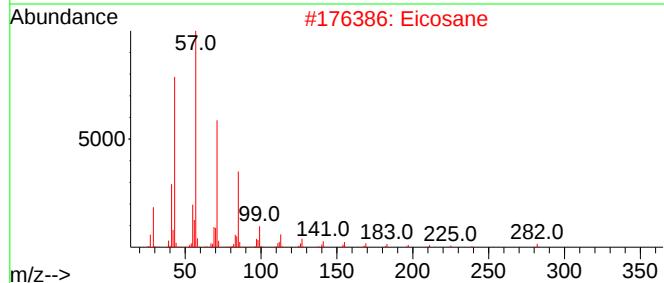
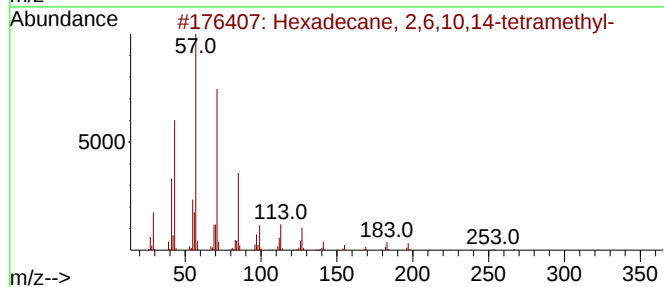
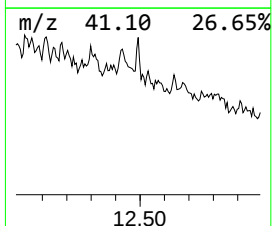
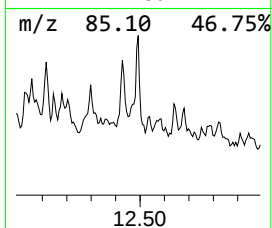
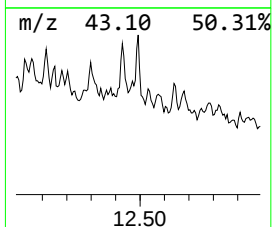
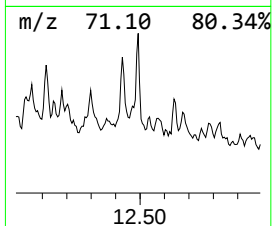
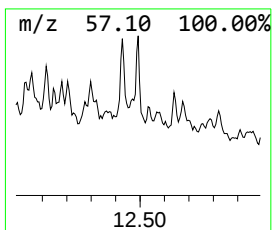
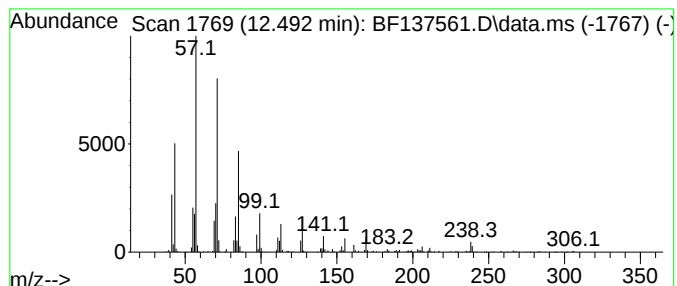
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane, 2,6,10,14-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	3.57 ng	324691	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
2		Eicosane	282	C20H42	000112-95-8	91
3		Pentacosane	352	C25H52	000629-99-2	87
4		Hentriacontane	437	C31H64	000630-04-6	87
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137561.D
Acq On : 11 Mar 2024 17:47
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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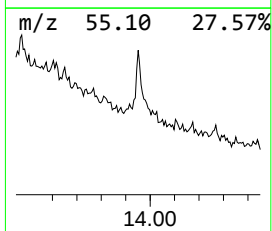
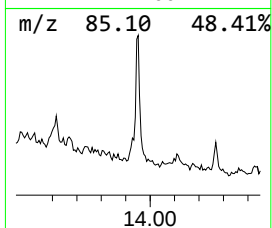
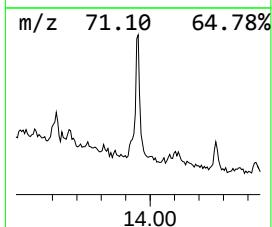
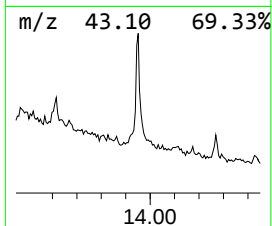
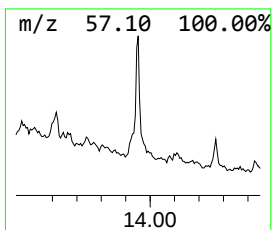
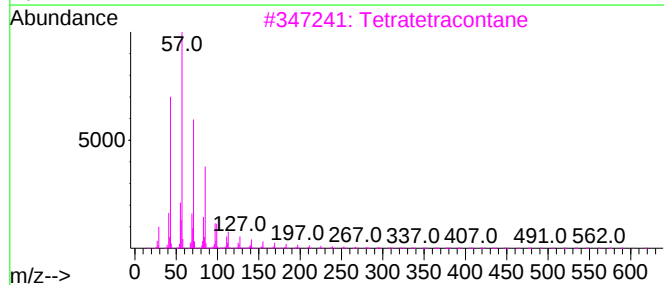
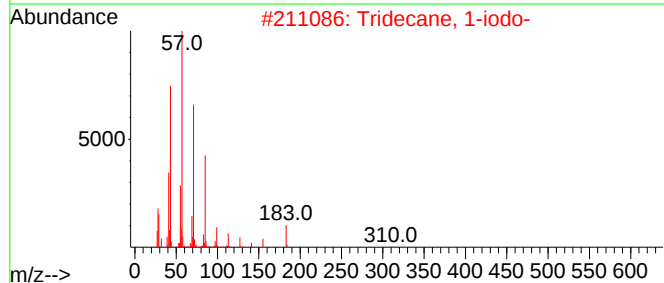
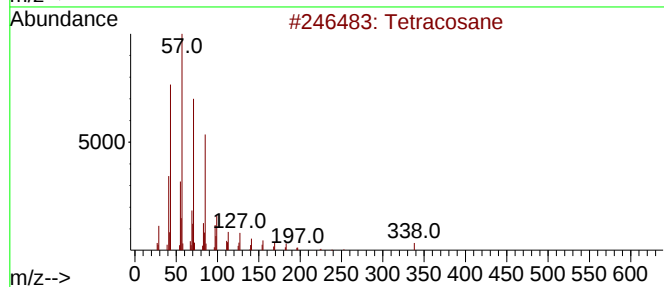
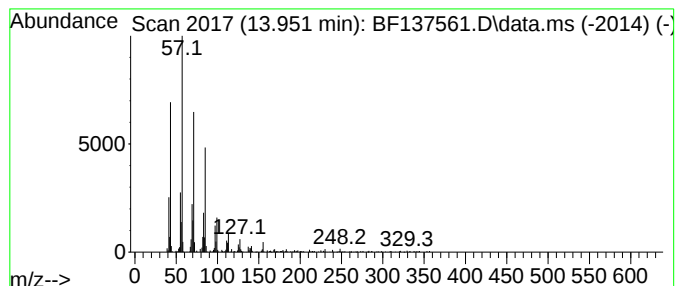
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	6.89 ng	498498	Chrysene-d12	14.092

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	93
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3		Tetratetracontane	619	C44H90	007098-22-8	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		2-Methylhexacosane	380	C27H56	001561-02-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
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Misc :
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Instrument :
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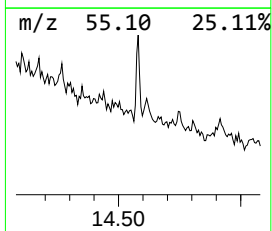
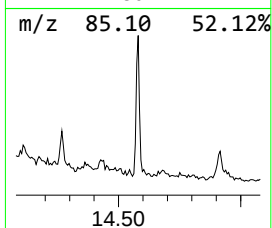
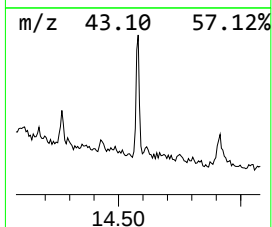
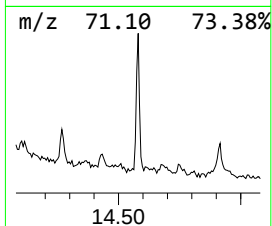
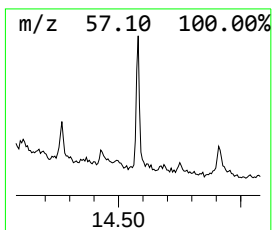
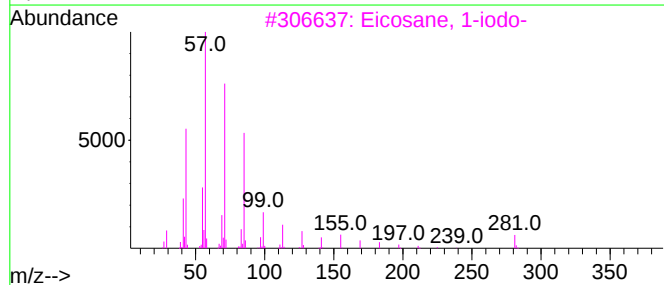
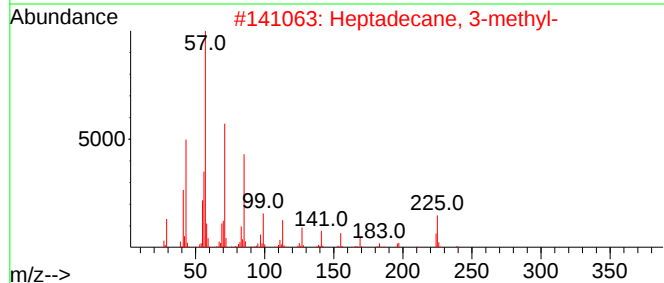
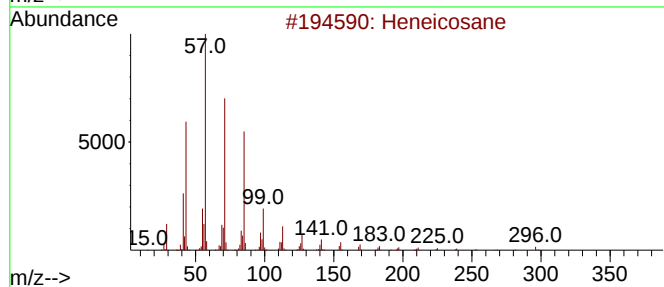
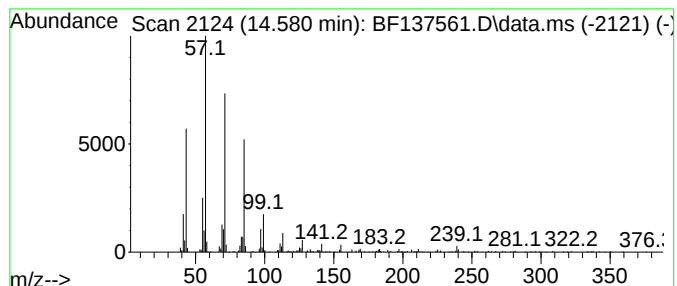
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	3.07 ng	222027	Chrysene-d12	14.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	86
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137561.D
Acq On : 11 Mar 2024 17:47
Operator : CG\JU
Sample : P1720-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT3471

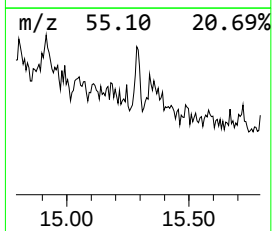
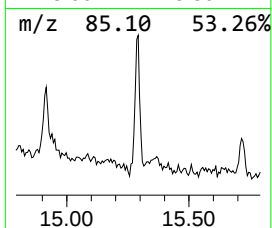
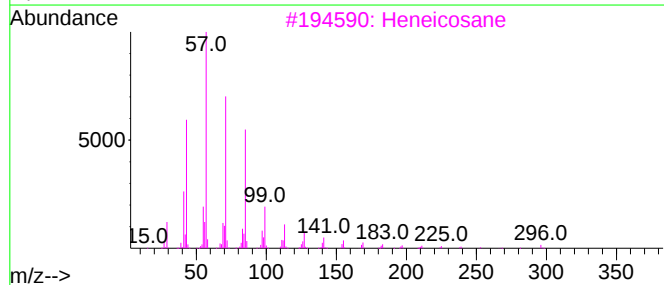
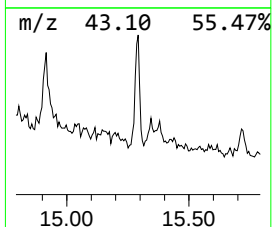
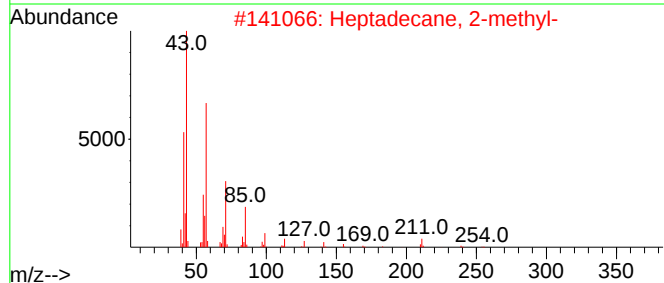
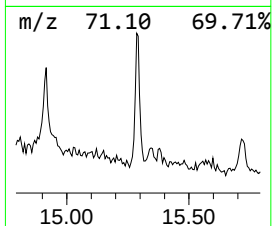
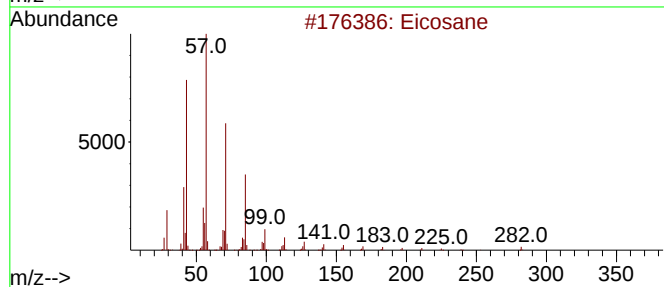
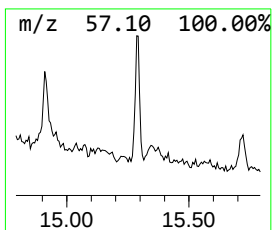
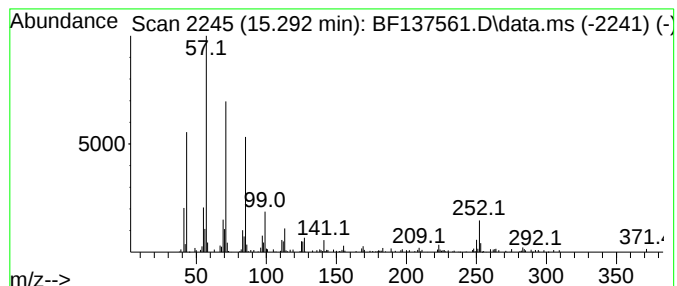
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.08 ng	131696	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	87
2			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	87
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
Data File : BF137561.D
Acq On : 11 Mar 2024 17:47
Operator : CG\JU
Sample : P1720-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT3471

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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...	2.281	21.2	ng	1447030	1	6.898	1364210	20.0
(1R)-2,6,6-Trim...	6.192	3.1	ng	214518	1	6.898	1364210	20.0
.beta.-Pinene	6.604	3.2	ng	216647	1	6.898	1364210	20.0
1-Dodecene	8.104	8.3	ng	789405	2	8.169	1902450	20.0
Undecane	10.592	3.0	ng	359661	3	9.928	2385670	20.0
Cyclopentane, 1...	10.804	3.1	ng	278953	4	11.427	1816800	20.0
Dodecane, 2,7,1...	10.863	8.0	ng	723886	4	11.427	1816800	20.0
unknown11.057	11.057	2.3	ng	209110	4	11.427	1816800	20.0
Hexacosane	11.333	13.5	ng	1226610	4	11.427	1816800	20.0
Hexadecane, 2,6...	12.492	3.6	ng	324691	4	11.427	1816800	20.0
Tetracosane	13.951	6.9	ng	498498	5	14.092	1447090	20.0
Heneicosane	14.580	3.1	ng	222027	5	14.092	1447090	20.0
Eicosane	15.292	2.1	ng	131696	6	15.645	1269280	20.0