

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
 Data File : BF137458.D
 Acq On : 01 Mar 2024 14:46
 Operator : CG\JU
 Sample : P1659-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-16

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: BF137458.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	8	15	26	rVB	1246546	1712882	44.94%	5.936%
2	5.134	514	518	525	rBV	55639	76051	2.00%	0.264%
3	5.522	580	584	606	rBV	4041638	3810454	99.98%	13.205%
4	6.510	748	752	770	rBV	3728714	3798183	99.66%	13.163%
5	6.869	810	813	823	rBV	1242724	1065532	27.96%	3.693%
6	7.428	904	908	921	rBV	2417883	2331546	61.18%	8.080%
7	8.139	1026	1029	1047	rBV	1471053	1370249	35.95%	4.749%
8	9.222	1209	1213	1216	rBV	4428393	3811234	100.00%	13.208%
9	9.898	1324	1328	1342	rBV	1653979	1389319	36.45%	4.815%
10	10.692	1459	1463	1477	rBV	1870668	1778266	46.66%	6.163%
11	11.392	1578	1582	1590	rBV	1317890	1153672	30.27%	3.998%
12	11.939	1672	1675	1688	rBV2	82709	128397	3.37%	0.445%
13	12.992	1850	1854	1858	rBV	3182745	3011674	79.02%	10.437%
14	13.910	2006	2010	2017	rBV	102395	153027	4.02%	0.530%
15	14.051	2030	2034	2048	rBV	1223798	1142251	29.97%	3.958%
16	14.268	2062	2071	2083	rVB8	58312	209776	5.50%	0.727%
17	14.951	2182	2187	2192	rBV	942686	982576	25.78%	3.405%
18	15.580	2289	2294	2304	rBV	665578	930853	24.42%	3.226%

Sum of corrected areas: 28855942

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

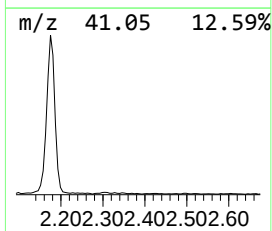
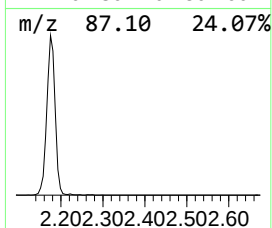
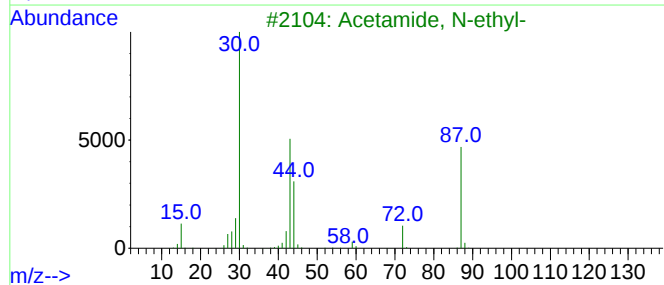
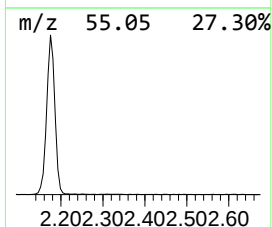
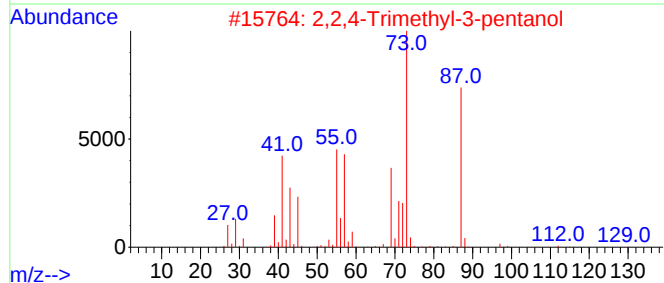
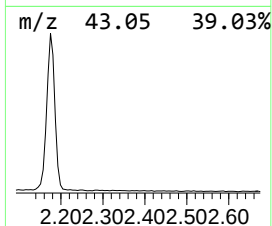
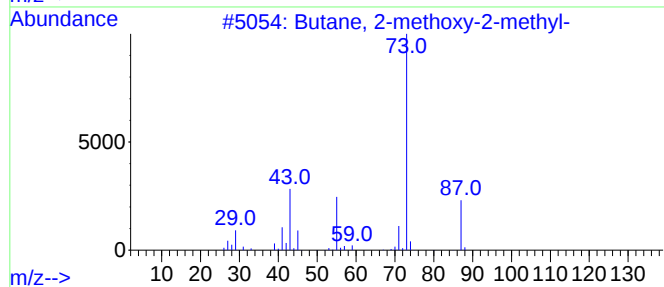
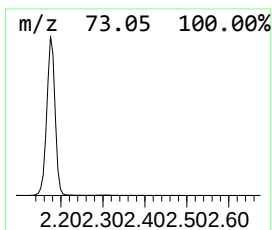
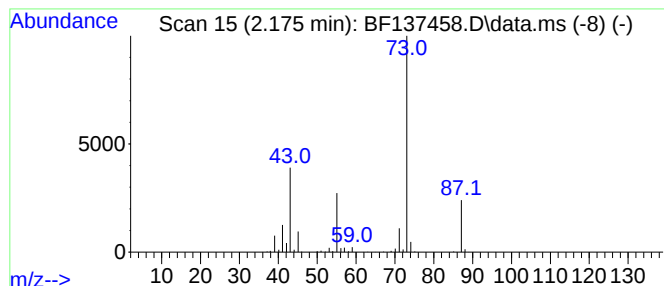
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	32.15 ng	1712880	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

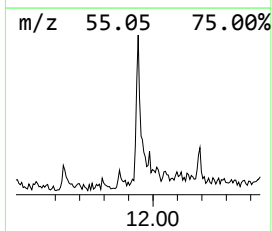
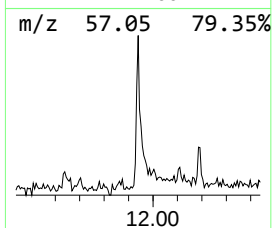
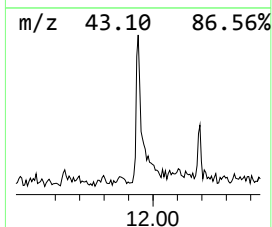
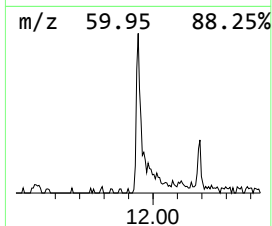
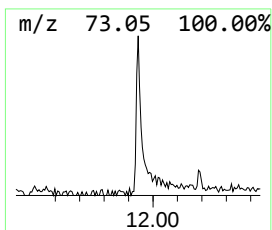
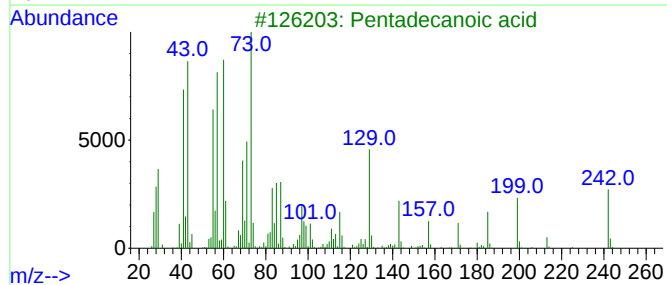
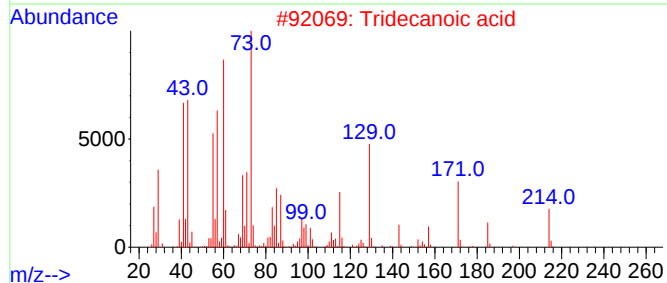
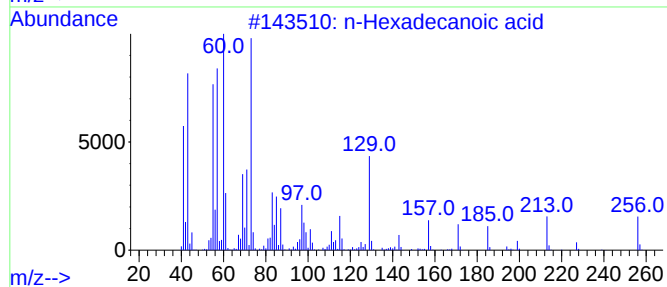
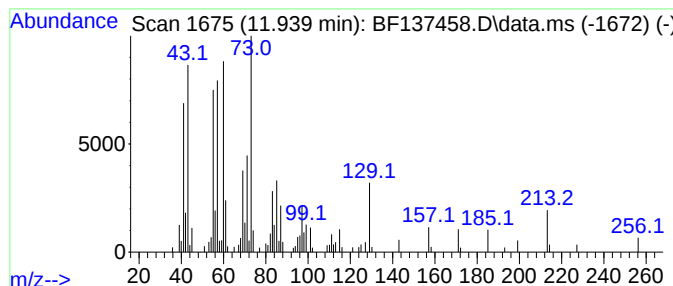
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.23 ng	128397	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64
5			d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

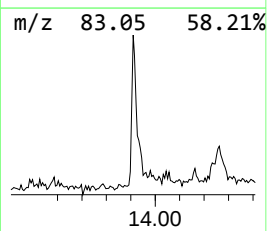
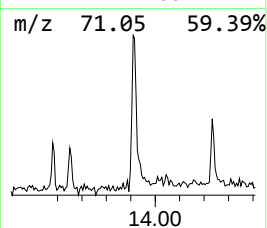
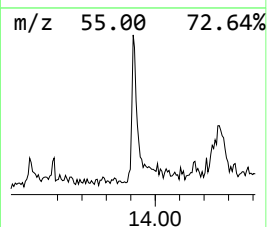
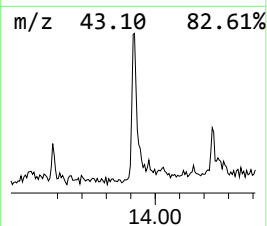
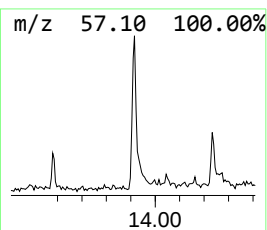
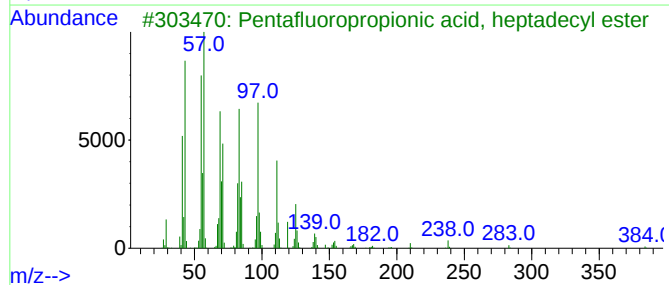
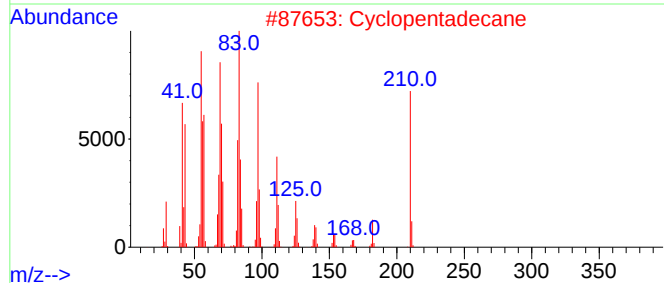
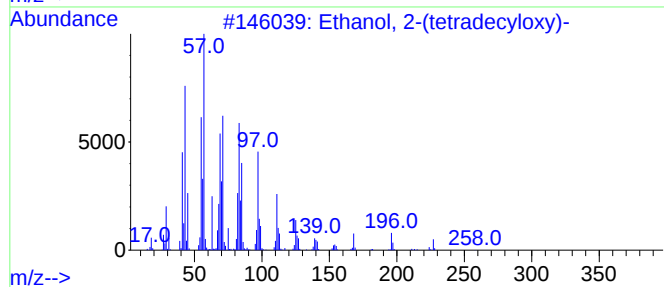
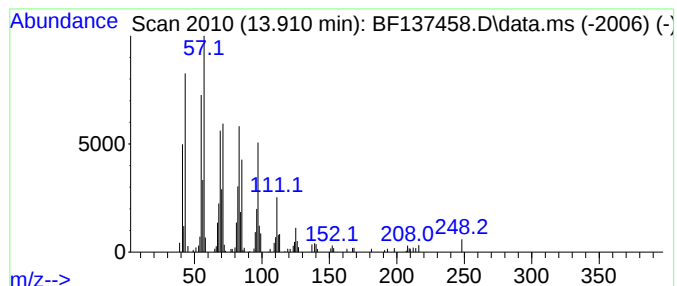
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.68 ng	153027	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2			Cyclopentadecane	210	C15H30	000295-48-7	86
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
5			1-Heptacosanol	396	C27H56O	002004-39-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

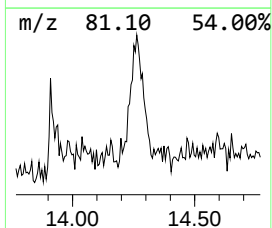
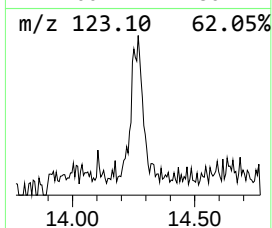
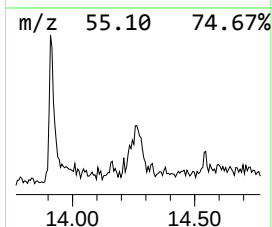
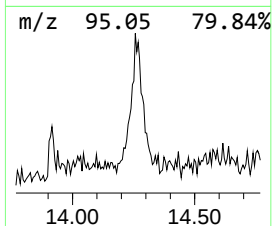
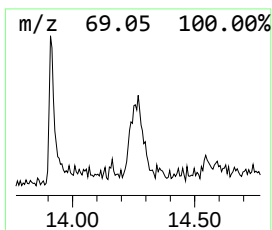
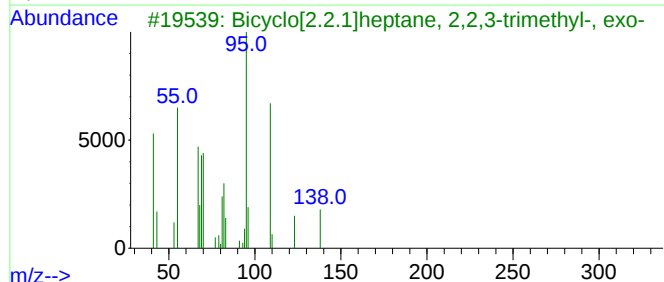
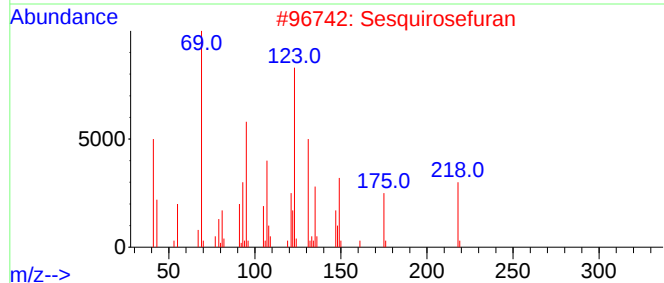
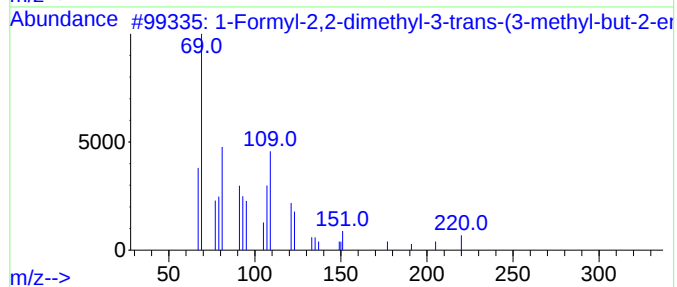
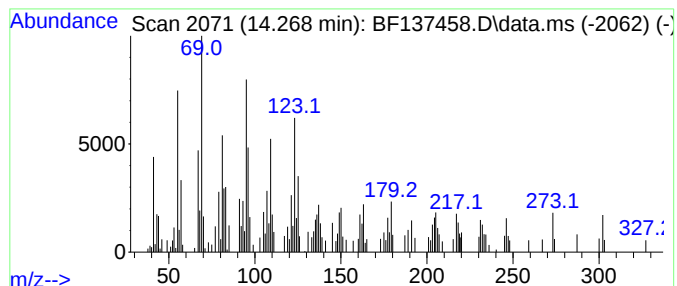
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown14.268 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	3.67 ng	209776	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	46
2			Sesquirosefuran	218	C15H22O	039007-93-7	46
3			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	42
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	42
5			Silane, monochloride, methylviny...	218	C10H19ClOSi	1000421-09-7	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

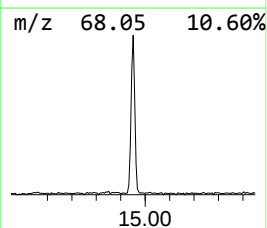
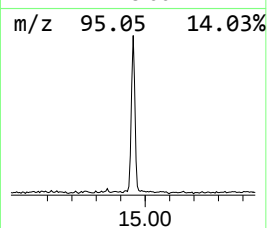
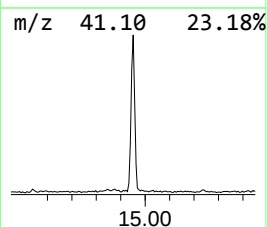
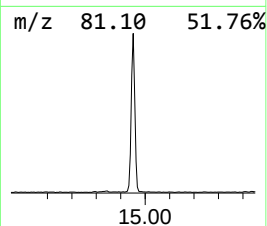
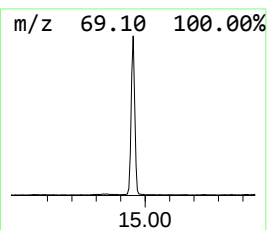
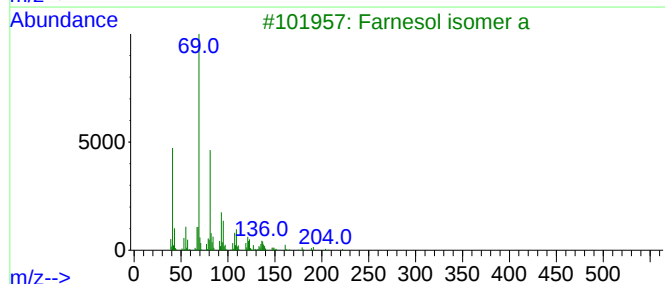
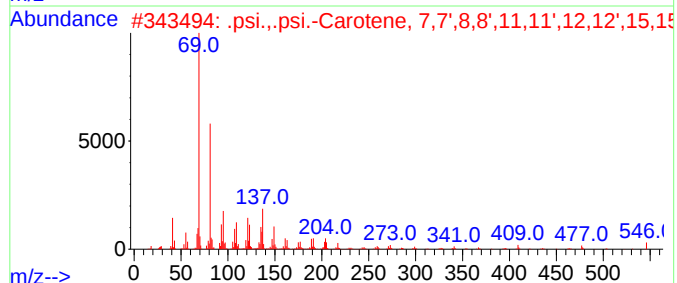
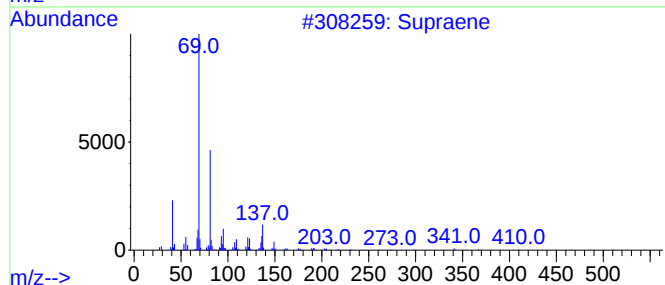
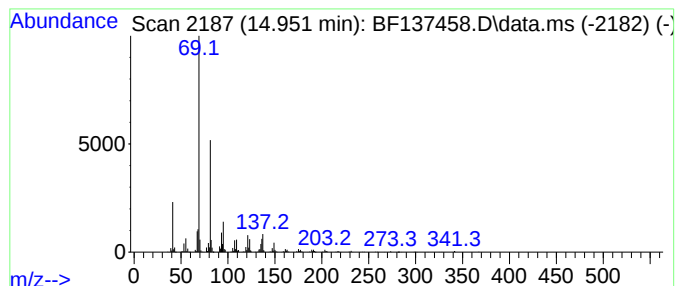
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	21.11 ng	982576	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
3			Farnesol isomer a	222	C15H26O	1000108-92-4	72
4			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	50
5			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030124\
Data File : BF137458.D
Acq On : 01 Mar 2024 14:46
Operator : CG\JU
Sample : P1659-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	32.1	ng	1712880	1	6.869	1065530	20.0
n-Hexadecanoic ...	11.939	2.2	ng	128397	4	11.392	1153670	20.0
Ethanol, 2-(tet...	13.910	2.7	ng	153027	5	14.051	1142250	20.0
unknown14.268	14.268	3.7	ng	209776	5	14.051	1142250	20.0
Supraene	14.951	21.1	ng	982576	6	15.580	930853	20.0