

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
 Data File : BF135720.D
 Acq On : 11 Oct 2023 18:45
 Operator : CG\JU
 Sample : 04791-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	9	19	21	rBV	17048	43288	1.97%	0.271%
2	4.963	486	489	500	rBV	373441	488159	22.23%	3.057%
3	5.375	556	559	580	rBV	1906543	2169909	98.82%	13.591%
4	6.392	728	732	752	rBV	1870747	2003134	91.23%	12.546%
5	6.740	788	791	796	rBV	537524	477341	21.74%	2.990%
6	7.304	883	887	901	rBV	1384654	1293773	58.92%	8.103%
7	8.016	1005	1008	1016	rBV	718722	627489	28.58%	3.930%
8	9.092	1187	1191	1201	rBV	2317652	2195815	100.00%	13.753%
9	9.216	1208	1212	1220	rVB	200824	229459	10.45%	1.437%
10	9.775	1303	1307	1321	rBV	853875	770776	35.10%	4.828%
11	10.569	1439	1442	1456	rBV	1155107	1147200	52.24%	7.185%
12	11.269	1558	1561	1570	rBV	832000	738721	33.64%	4.627%
13	11.804	1649	1652	1665	rBV4	87437	134840	6.14%	0.845%
14	12.492	1766	1769	1775	rBV	127352	126210	5.75%	0.790%
15	12.598	1785	1787	1793	rBV5	15021	27285	1.24%	0.171%
16	12.727	1803	1809	1813	rBV	106140	123483	5.62%	0.773%
17	12.863	1828	1832	1836	rBV	1965532	1793292	81.67%	11.232%
18	13.898	1998	2008	2010	rBV6	24119	71472	3.25%	0.448%
19	13.933	2010	2014	2017	rVV	498388	515220	23.46%	3.227%
20	13.963	2017	2019	2023	rVB	47893	48258	2.20%	0.302%
21	14.768	2152	2156	2161	rVB	149458	143543	6.54%	0.899%
22	14.986	2189	2193	2196	rBV	39343	63321	2.88%	0.397%
23	15.286	2241	2244	2248	rBV2	24919	30846	1.40%	0.193%
24	15.351	2252	2255	2260	rVV	43099	52322	2.38%	0.328%
25	15.404	2260	2264	2273	rVB	429702	572017	26.05%	3.583%
26	15.839	2335	2338	2342	rBV2	21275	29035	1.32%	0.182%
27	16.927	2519	2523	2529	rBV6	22654	49965	2.28%	0.313%

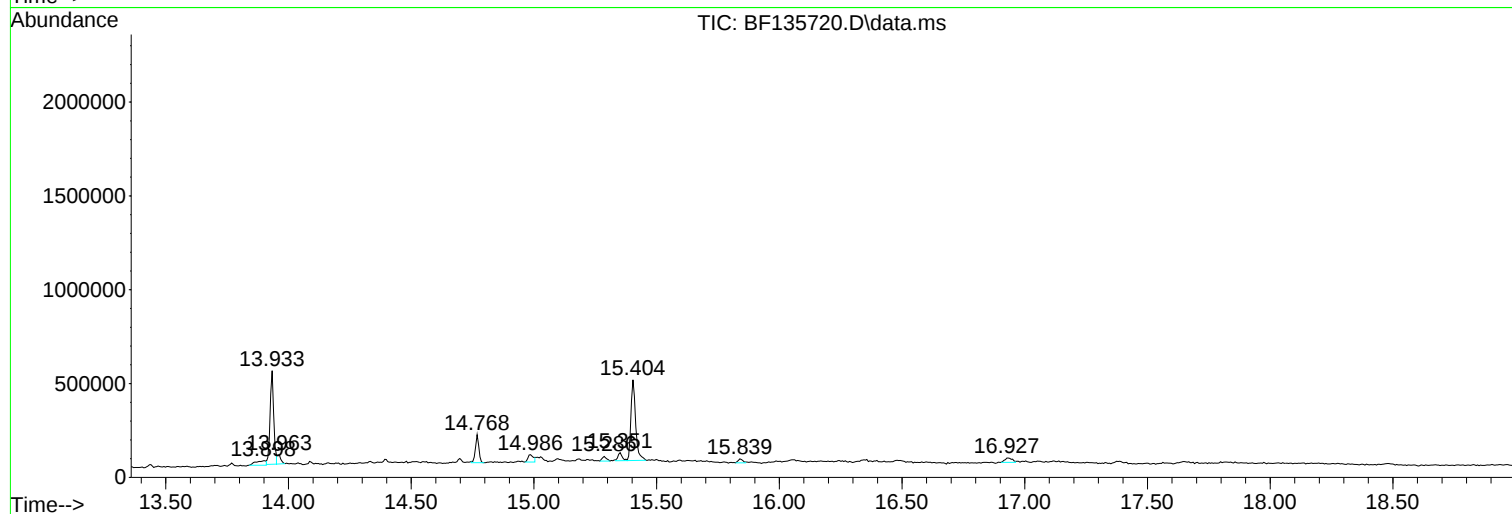
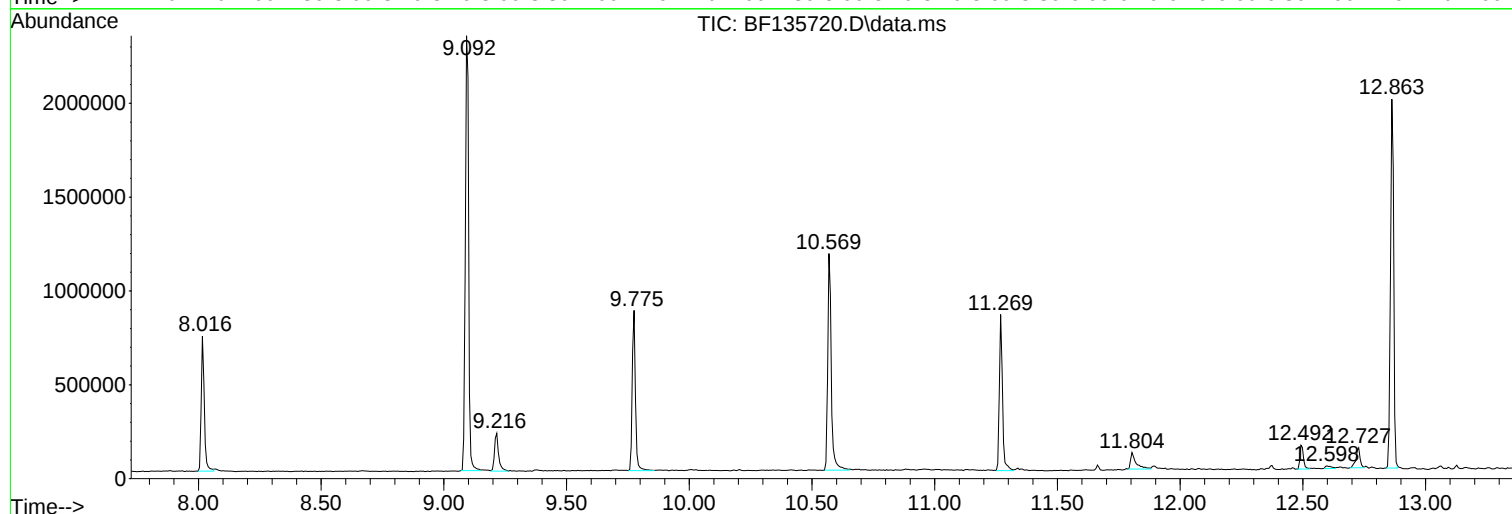
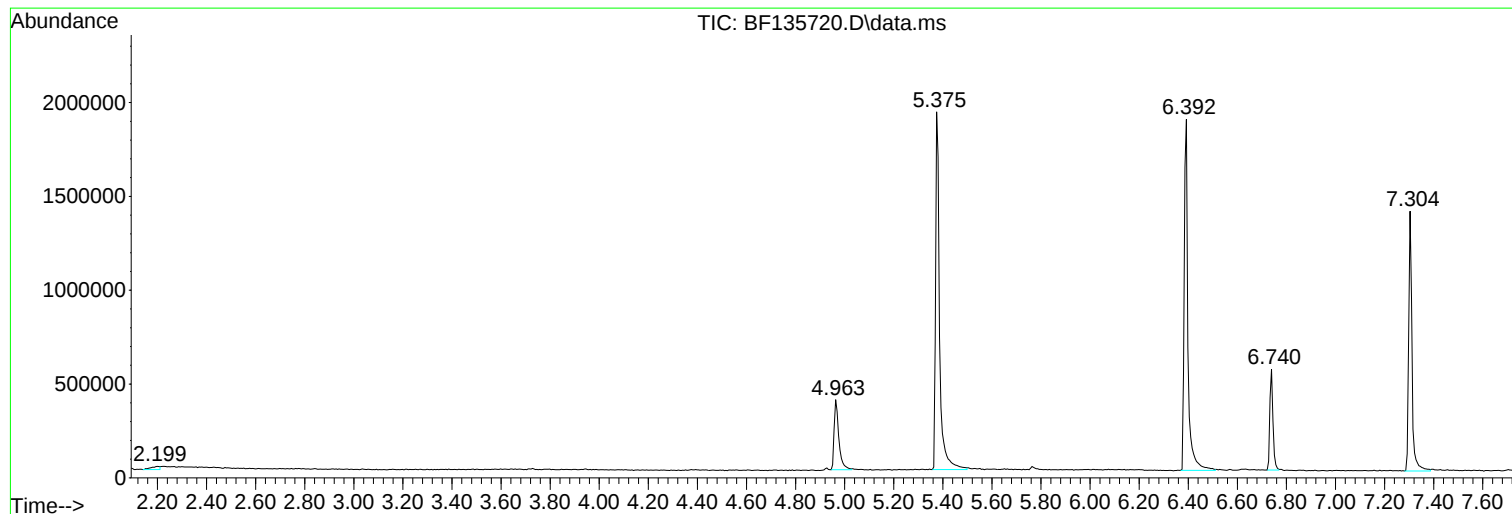
Sum of corrected areas: 15966173

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

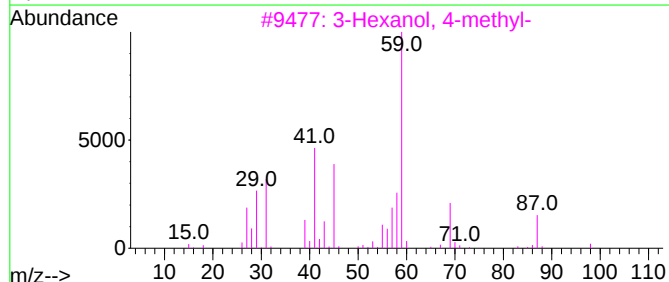
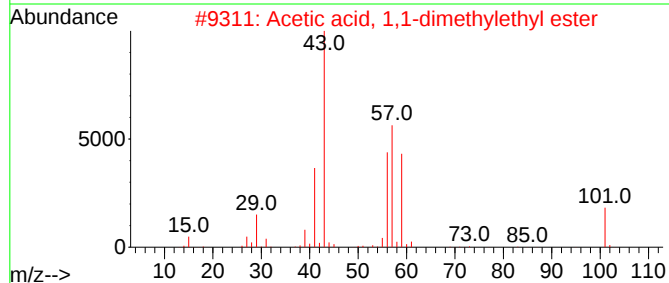
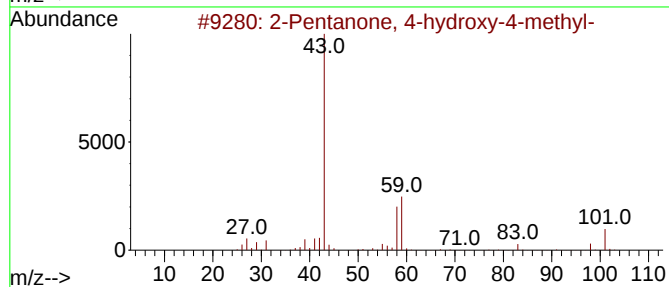
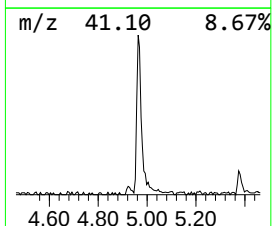
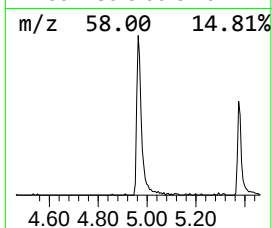
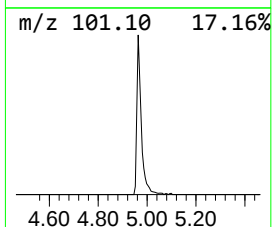
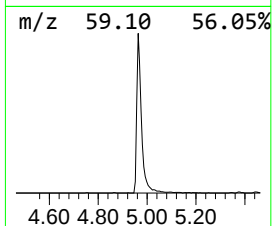
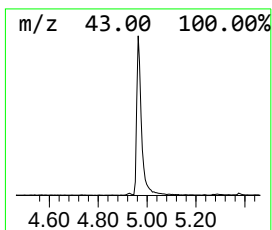
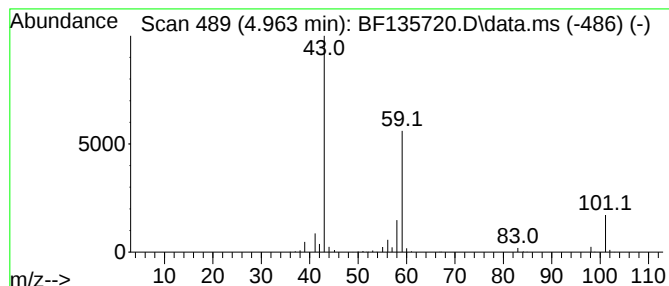
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	20.45 ng	488159	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

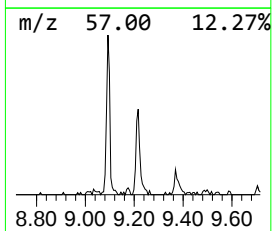
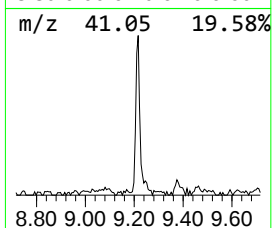
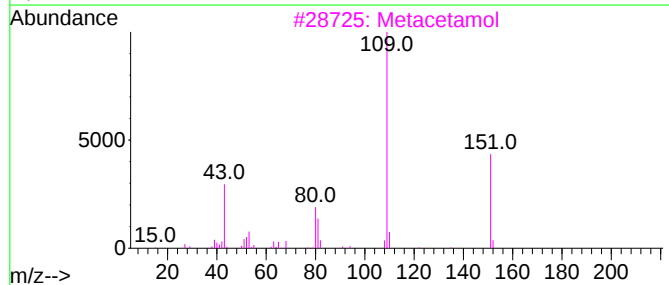
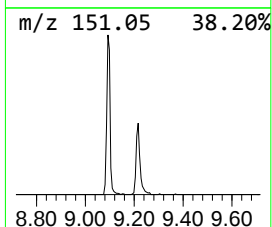
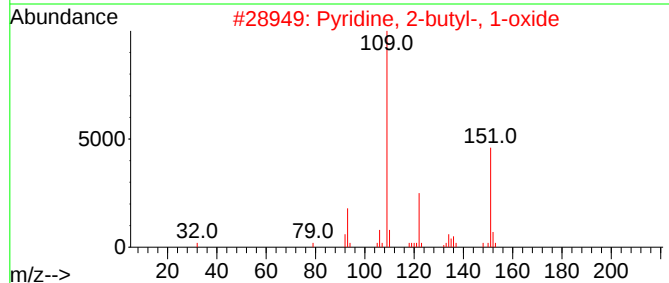
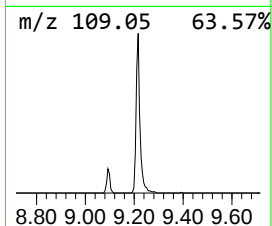
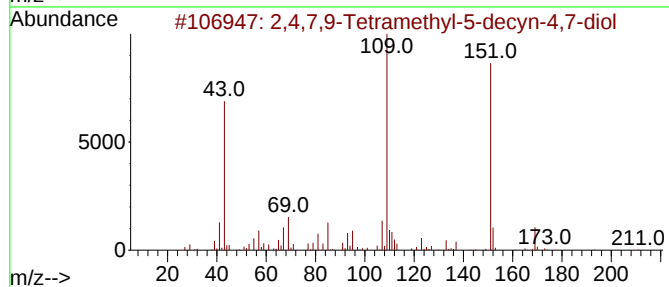
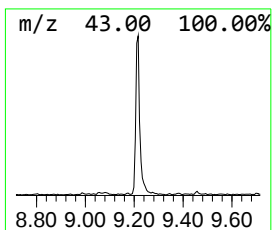
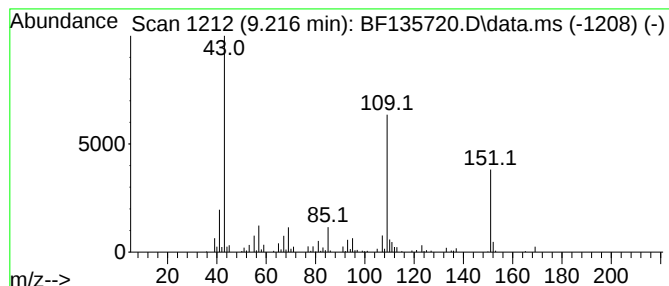
Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.216	5.95 ng	229459	Acenaphthene-d10			9.775
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	90
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	Metacetamol		151	C8H9NO2	000621-42-1	53
4	Acetaminophen		151	C8H9NO2	000103-90-2	53
5	m-Isopropoxyaniline		151	C9H13NO	041406-00-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

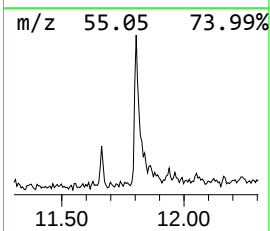
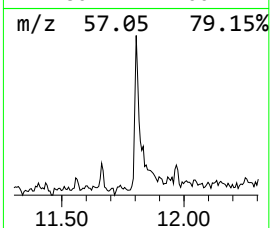
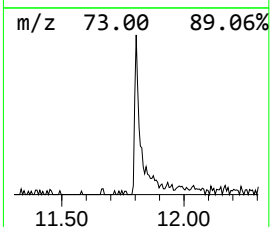
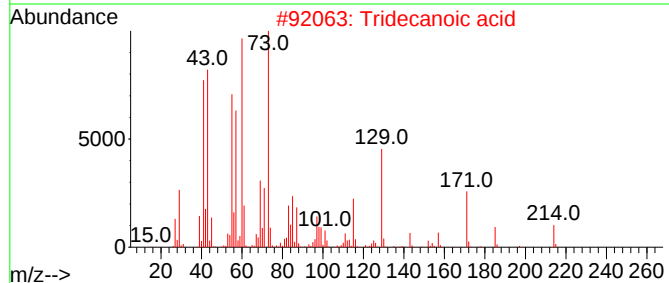
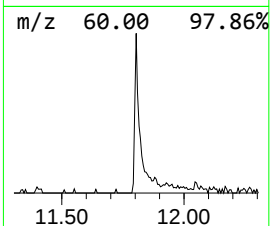
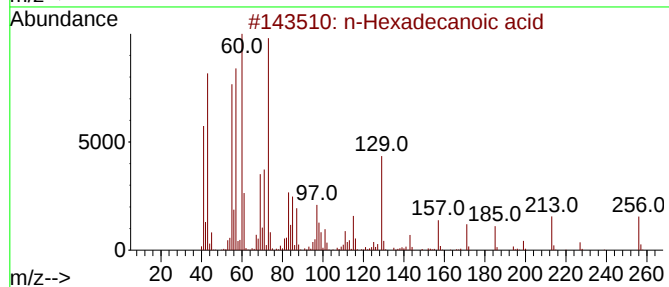
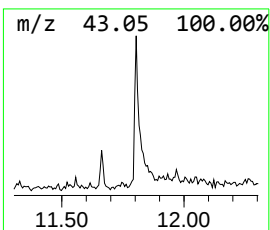
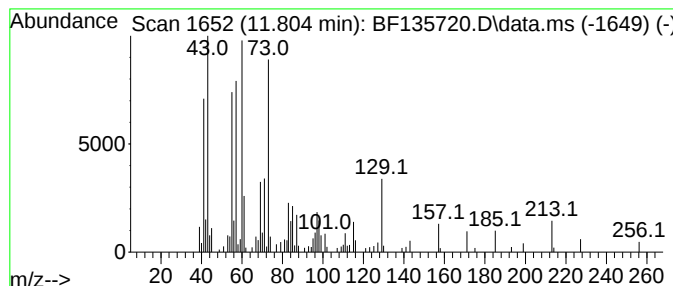
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.65 ng	134840	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

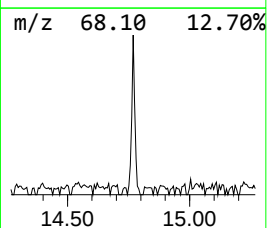
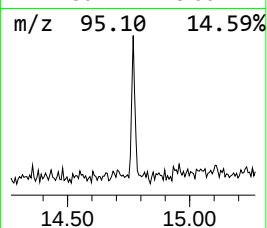
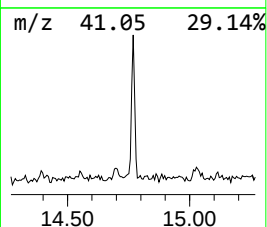
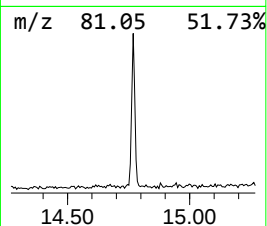
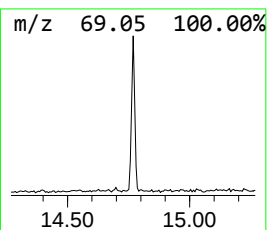
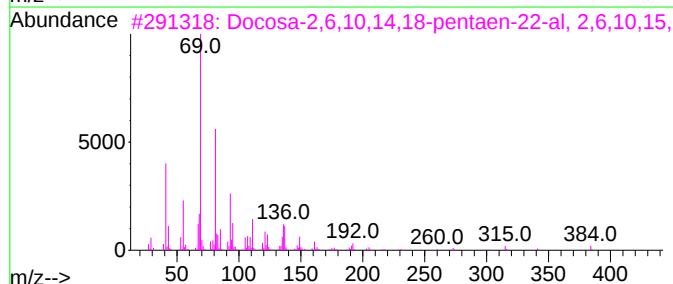
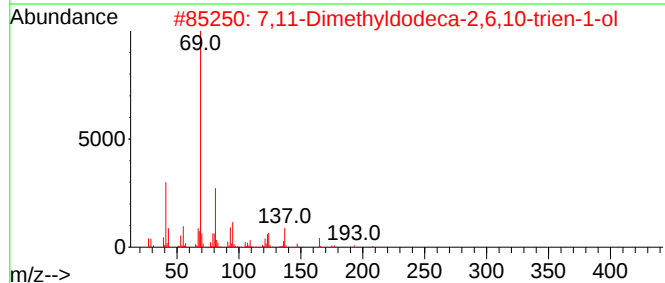
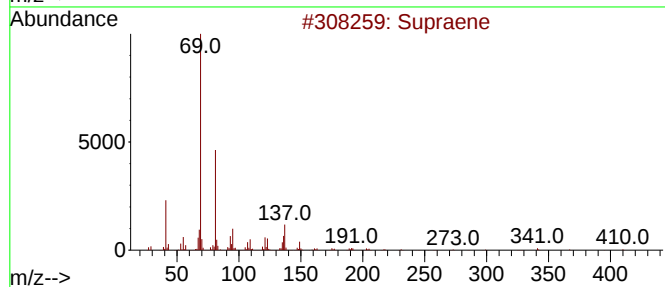
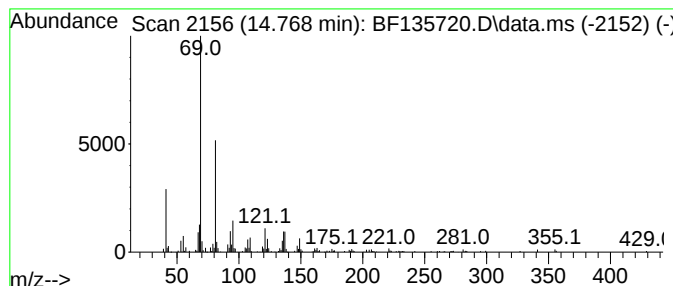
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	5.02 ng	143543	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	81
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	72
5			Farnesol isomer a	222	C15H26O	1000108-92-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135720.D
Acq On : 11 Oct 2023 18:45
Operator : CG\JU
Sample : 04791-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
2-Pentanone, 4-...	4.963	20.4	ng	488159	1	6.740	477341	20.0
2,4,7,9-Tetrame...	9.216	6.0	ng	229459	3	9.775	770776	20.0
n-Hexadecanoic ...	11.804	3.6	ng	134840	4	11.269	738721	20.0
Supraene	14.768	5.0	ng	143543	6	15.404	572017	20.0