

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072120\
 Data File : BF120956.D
 Acq On : 21 Jul 2020 16:14
 Operator : JU/CG
 Sample : L3358-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 55-ST-28

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF071620.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	563	567	577	rBV	1281449	1136019	23.21%	3.556%
2	6.434	736	739	750	rVB	776409	694250	14.18%	2.173%
3	6.645	771	775	783	rBV	129815	145856	2.98%	0.457%
4	6.816	800	804	807	rBV	1131728	987536	20.17%	3.091%
5	6.969	826	830	834	rBV	3236772	3154671	64.45%	9.875%
6	7.381	890	900	903	rBV	2457029	2638254	53.90%	8.258%
7	7.845	970	979	982	rBV	34239	60467	1.24%	0.189%
8	7.904	982	989	990	rBV4	54274	78334	1.60%	0.245%
9	7.928	990	993	996	rVB	81486	87803	1.79%	0.275%
10	8.022	1002	1009	1011	rBV2	149900	252394	5.16%	0.790%
11	8.098	1018	1022	1030	rVB	1457981	1455080	29.73%	4.555%
12	8.239	1042	1046	1050	rVB5	71803	86015	1.76%	0.269%
13	8.369	1064	1068	1074	rVB4	47668	75167	1.54%	0.235%
14	8.469	1074	1085	1088	rBV2	103581	220038	4.50%	0.689%
15	8.545	1096	1098	1102	rVB	75927	71396	1.46%	0.223%
16	9.175	1200	1205	1208	rBV	4501337	4697548	95.96%	14.705%
17	9.292	1219	1225	1240	rVB	1067558	1095475	22.38%	3.429%
18	9.563	1268	1271	1277	rBV	588645	534715	10.92%	1.674%
19	9.851	1316	1320	1327	rVB	1652953	1518251	31.02%	4.753%
20	10.439	1417	1420	1425	rBV	229386	260836	5.33%	0.816%
21	10.639	1449	1454	1460	rBV	2264894	2304779	47.08%	7.215%
22	11.333	1568	1572	1576	rBV	1808716	1563023	31.93%	4.893%
23	11.869	1659	1663	1666	rBV	115338	109839	2.24%	0.344%
24	12.404	1750	1754	1763	rBV2	80915	120520	2.46%	0.377%
25	12.580	1779	1784	1787	rBV	103188	98042	2.00%	0.307%
26	12.921	1837	1842	1846	rBV	4170327	4895128	100.00%	15.323%
27	13.833	1993	1997	2009	rBV	332361	469653	9.59%	1.470%
28	13.968	2016	2020	2034	rVB	1707865	1519049	31.03%	4.755%
29	14.821	2161	2165	2170	rBV	151231	145238	2.97%	0.455%
30	15.080	2205	2209	2214	rVB	41977	50097	1.02%	0.157%
31	15.415	2260	2266	2271	rBV	1047429	1308523	26.73%	4.096%
32	15.880	2341	2345	2353	rVB2	34745	50222	1.03%	0.157%
33	15.968	2355	2360	2368	rBV7	23018	61972	1.27%	0.194%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-28

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

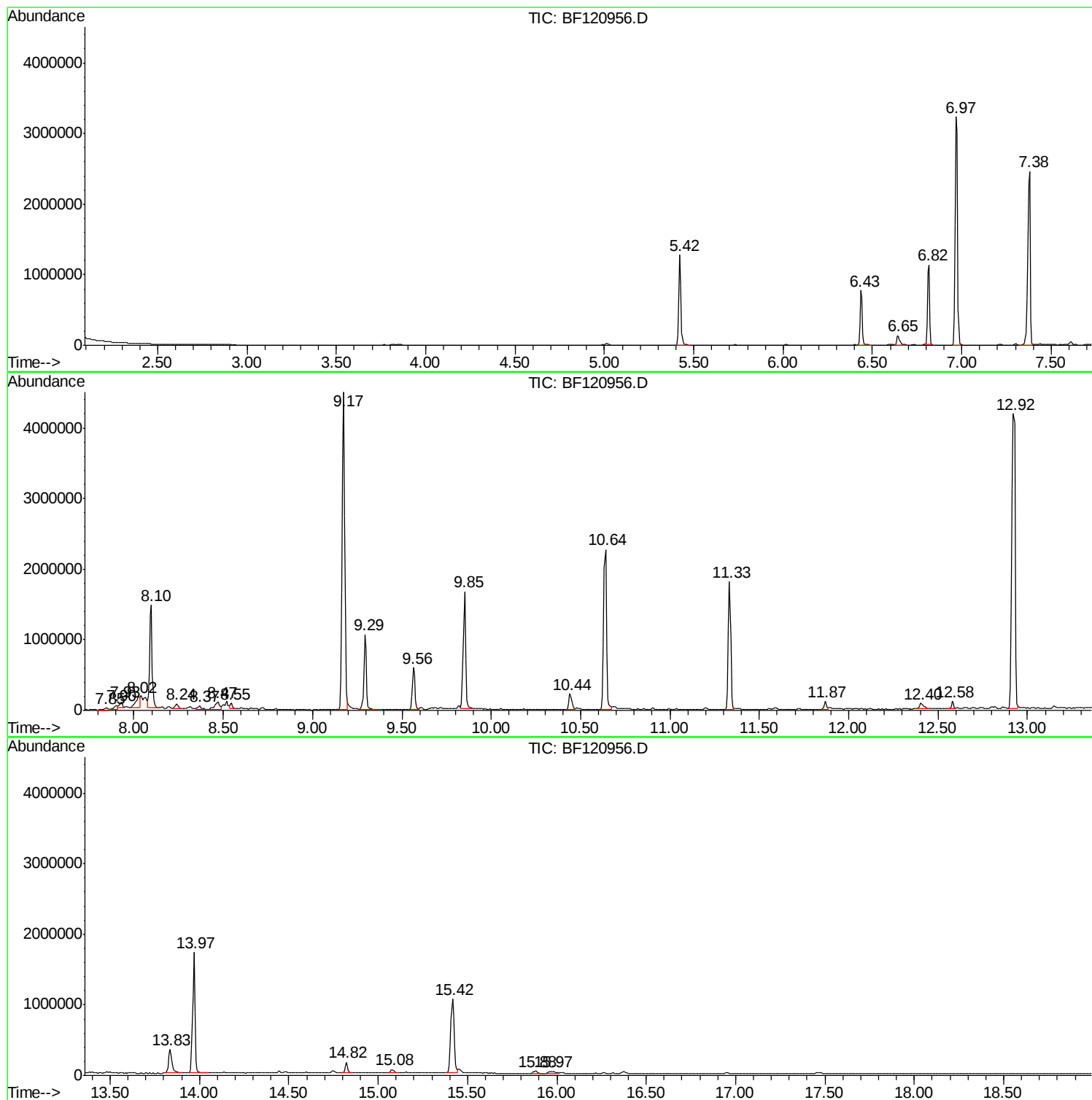
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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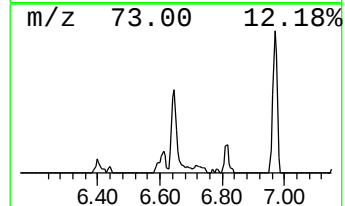
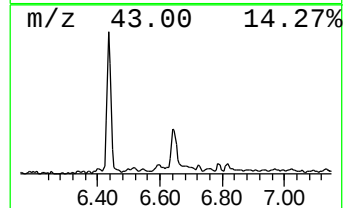
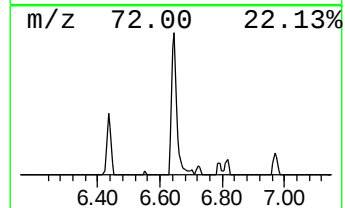
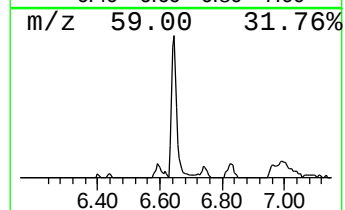
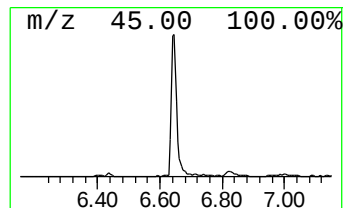
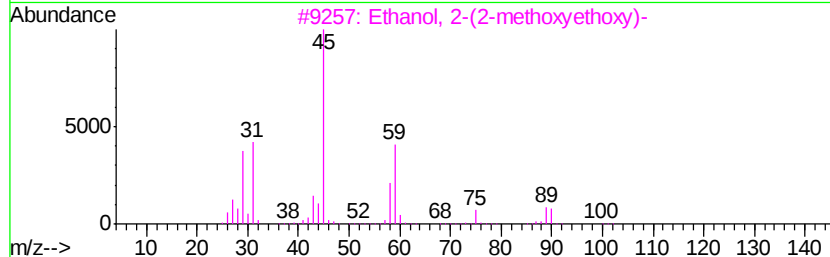
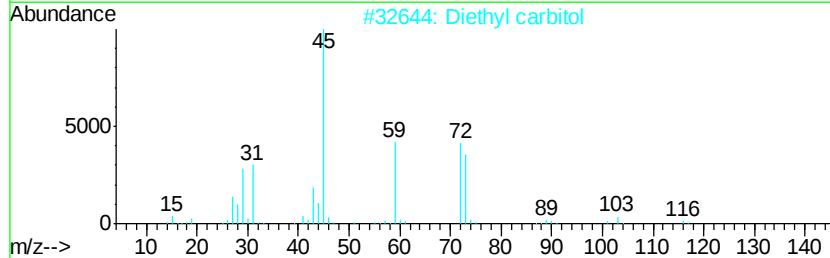
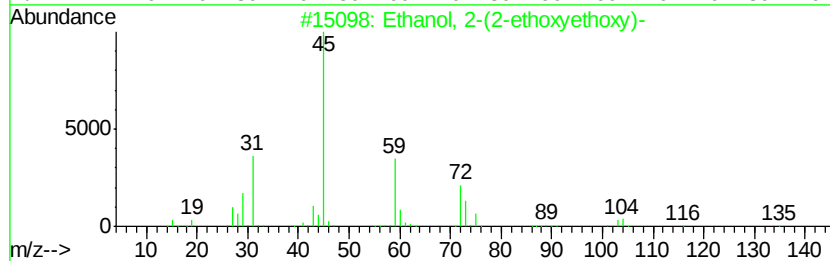
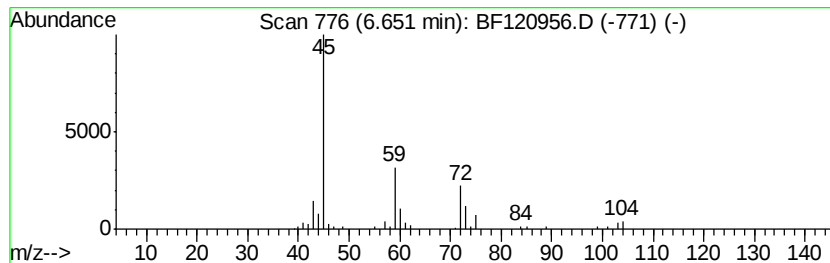
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	2.95 ng	145856	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2		Diethyl carbitol	162	C8H18O3	000112-36-7	72
3		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
4		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5		Ethanol, 2-[2-(2-ethoxyethoxy)et...]	178	C8H18O4	000112-50-5	38



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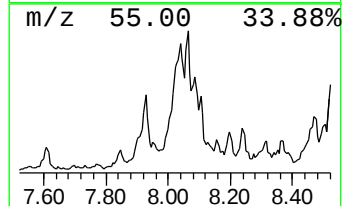
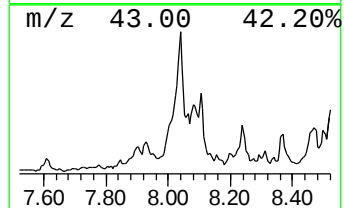
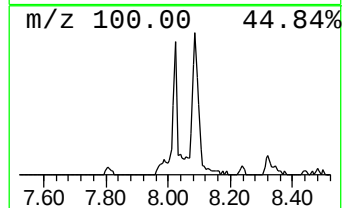
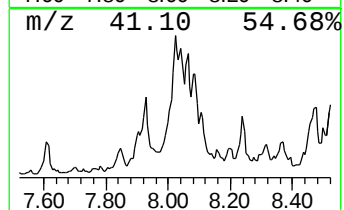
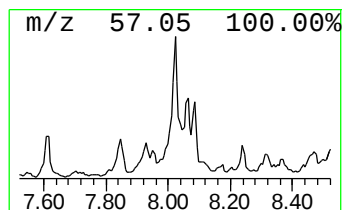
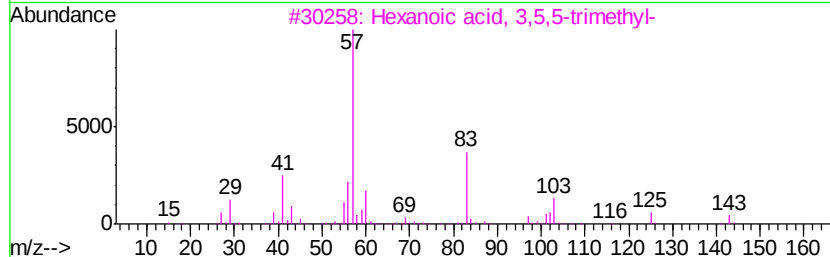
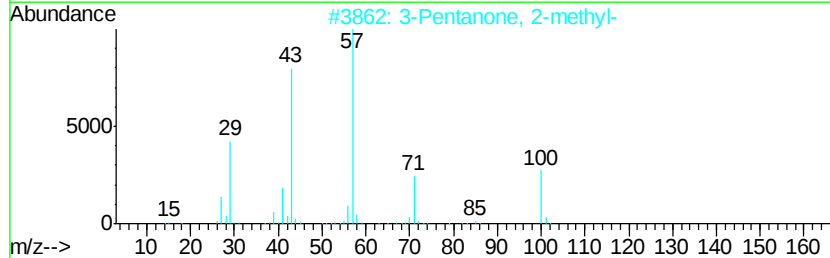
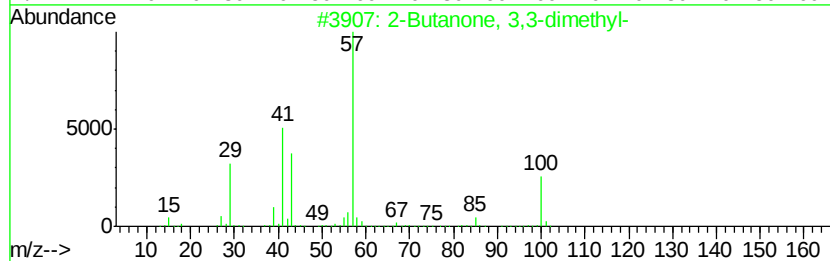
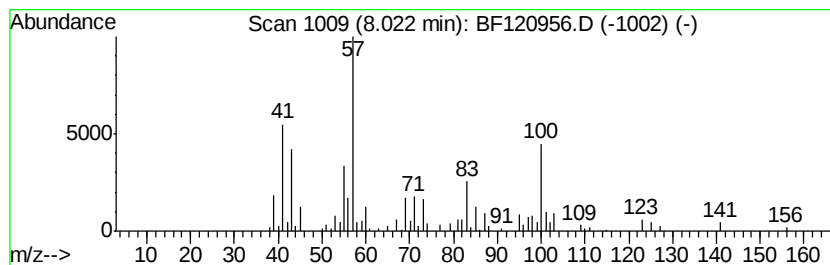
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	3.47 ng	252394	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	43
2		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	38
3		Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	35
4		2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	22
5		Cyclohexyl isovalerate	184	C11H20O2	007774-44-9	16



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Misc :
ALS Vial : 12 Sample Multiplier: 1

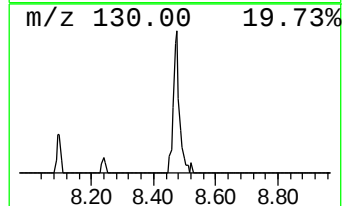
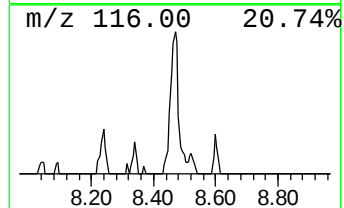
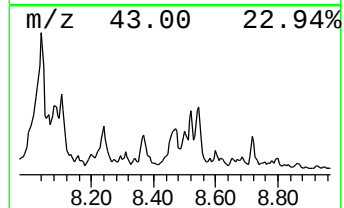
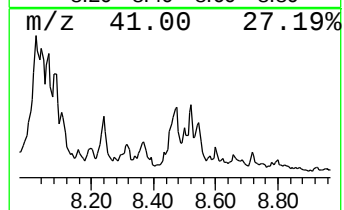
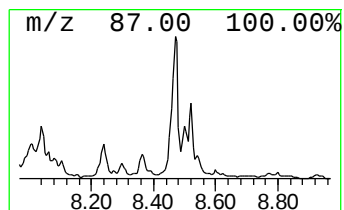
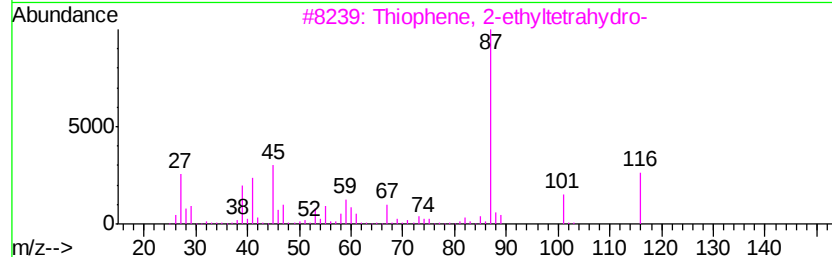
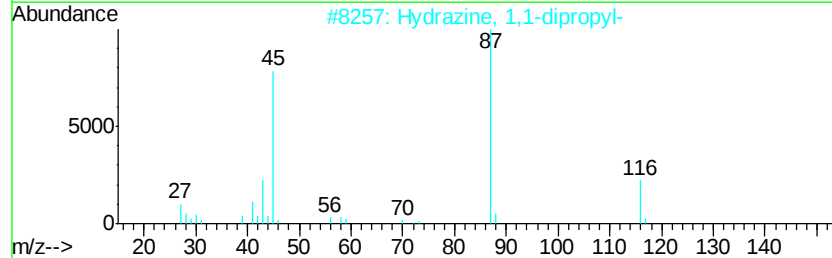
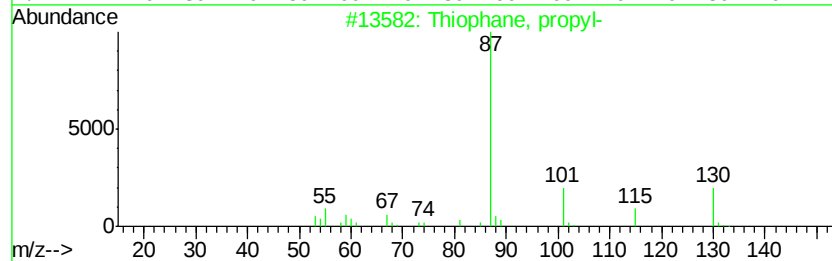
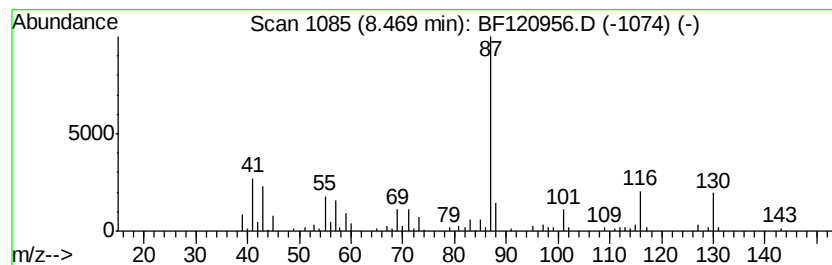
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophane, propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	3.02 ng	220038	Naphthalene-d8	8.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Thiophane, propyl-	130 C7H14S	001551-34-4 53
2		Hydrazine, 1,1-dipropyl-	116 C6H16N2	004986-50-9 49
3		Thiophene, 2-ethyltetrahydro-	116 C6H12S	001551-32-2 45
4		Ethanol, 2,2'-[1,2-ethanediylbis...	234 C10H18O6	000111-21-7 43
5		2-[2-[2-[2-[2-[2-[2-[2-(2-Ace...	542 C24H46O13	1000351-90-4 43



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Data File : BF120956.D
Acq On : 21 Jul 2020 16:14
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Sample : L3358-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-28

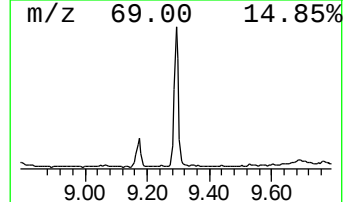
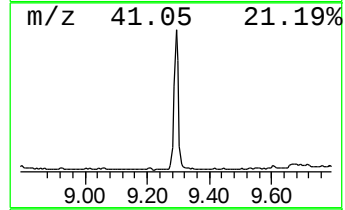
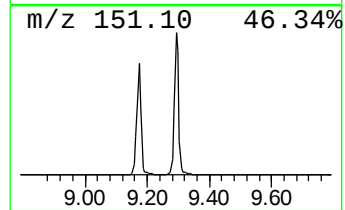
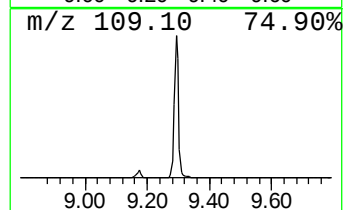
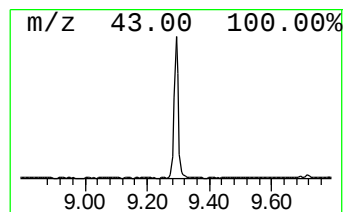
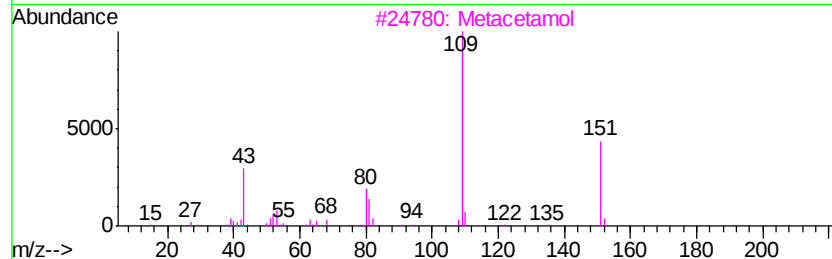
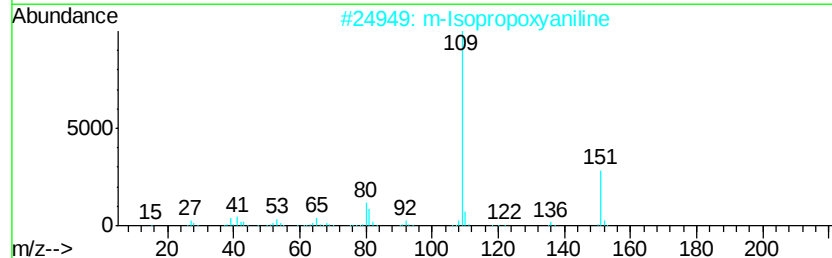
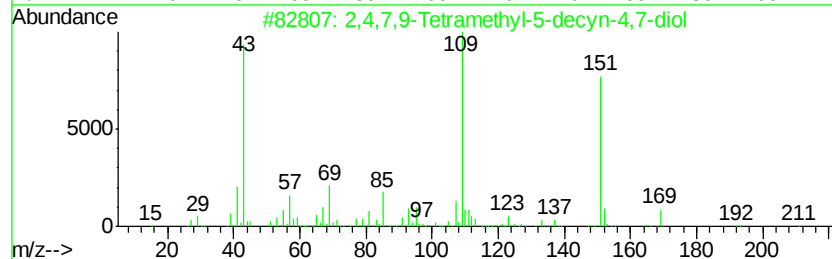
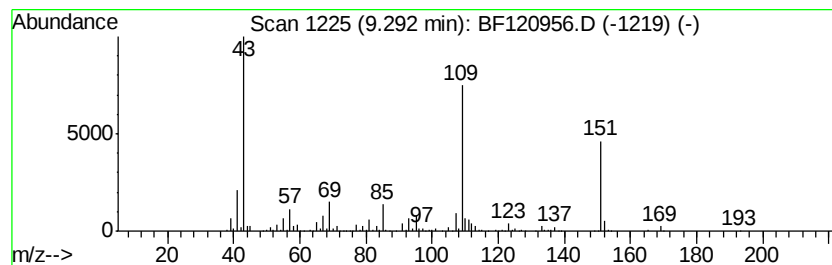
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	14.43 ng	1095480	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
3		Metacetamol	151	C8H9NO2	000621-42-1	59
4		3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
5		Acetaminophen	151	C8H9NO2	000103-90-2	59



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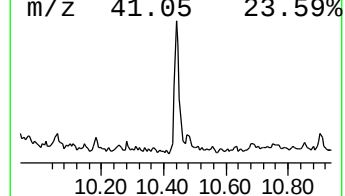
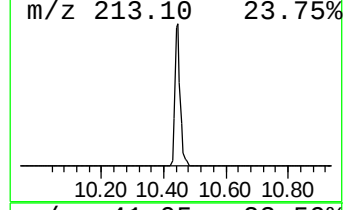
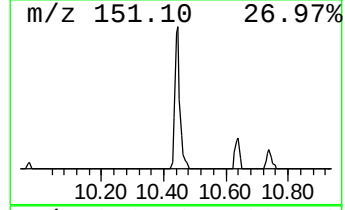
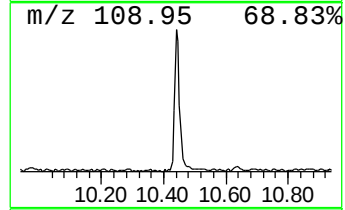
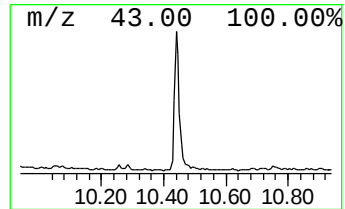
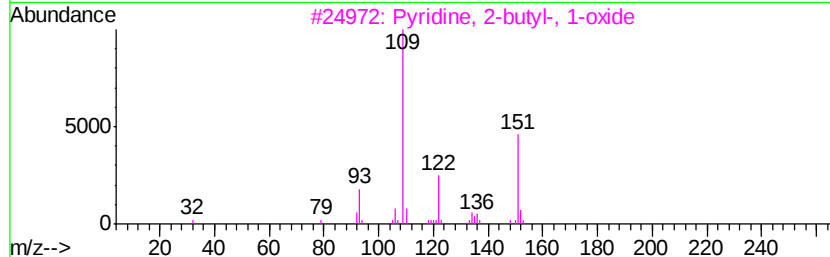
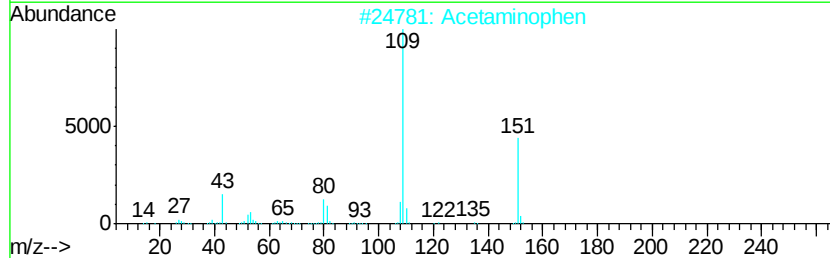
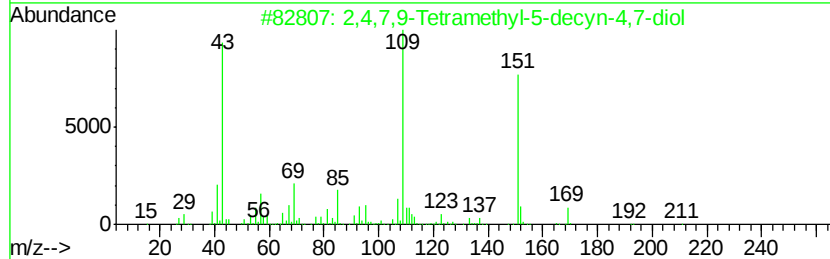
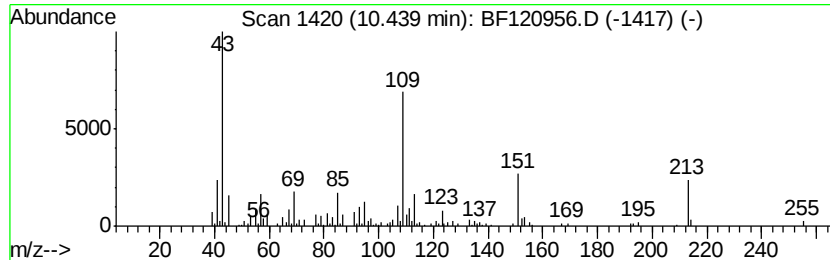
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Peak Number 6 unknown10.44 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.44	3.44 ng	260836	Acenaphthene-d10	9.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	64
2	Acetaminophen	151	C8H9NO2	000103-90-2	38
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	35
4	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	35
5	Metacetamol	151	C8H9NO2	000621-42-1	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072120\
Data File : BF120956.D
Acq On : 21 Jul 2020 16:14
Operator : JU/CG
Sample : L3358-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-28

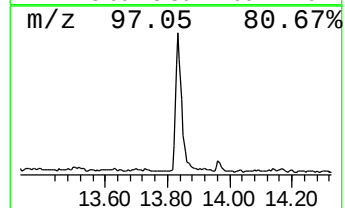
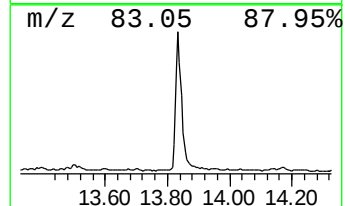
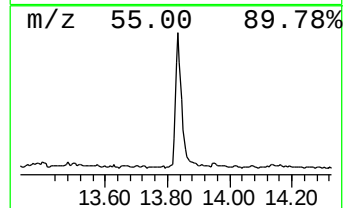
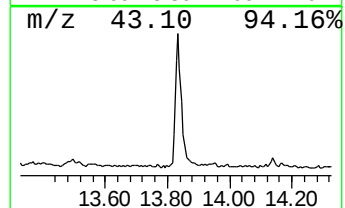
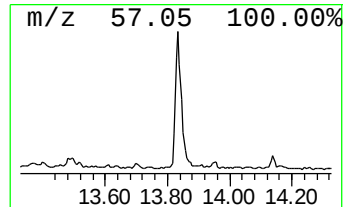
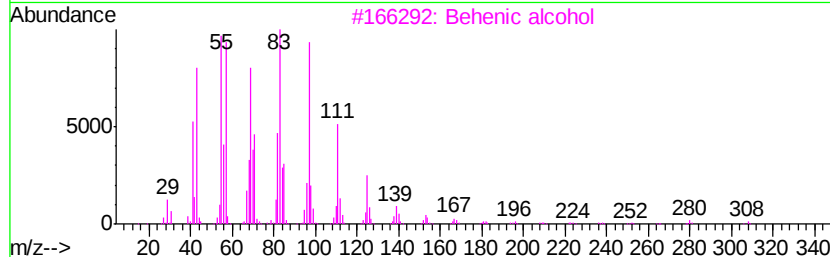
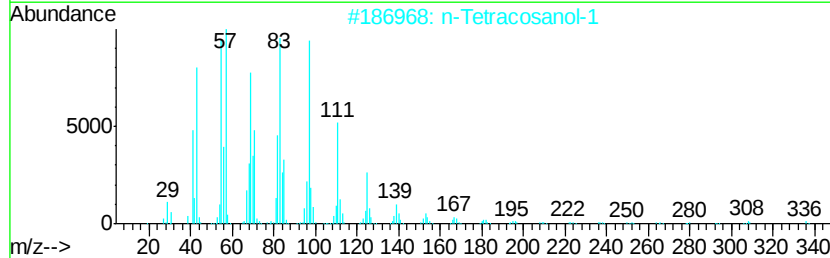
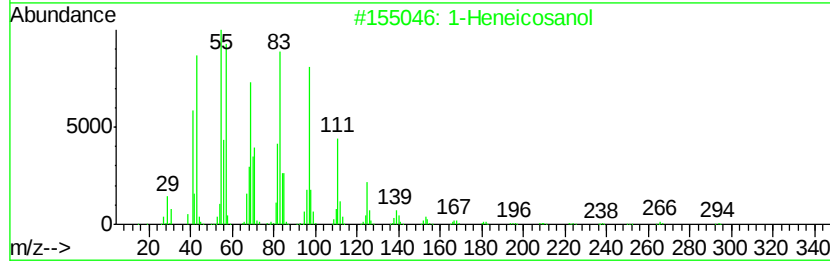
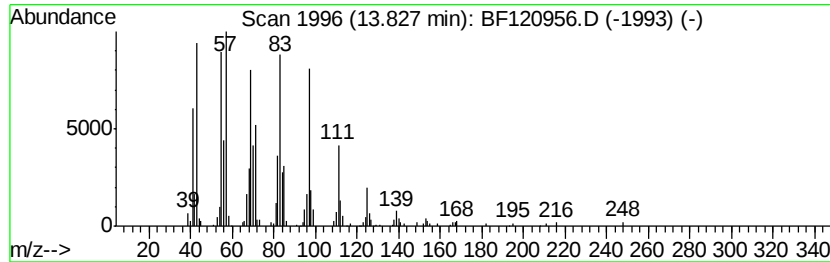
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.18 ng	469653	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		Behenic alcohol	326	C22H46O	000661-19-8	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072120\
Data File : BF120956.D
Acq On : 21 Jul 2020 16:14
Operator : JU/CG
Sample : L3358-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-28

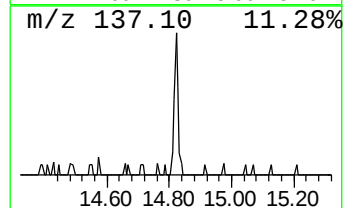
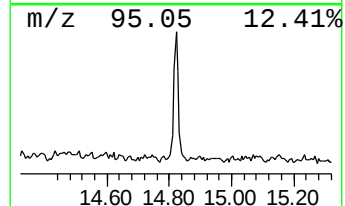
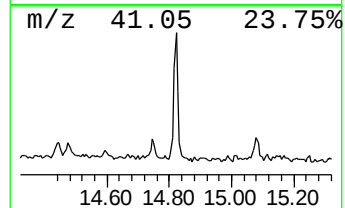
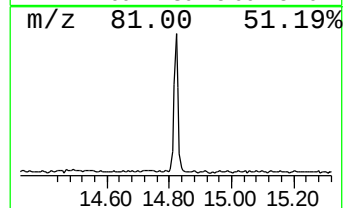
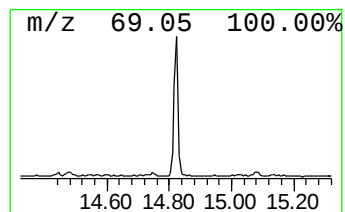
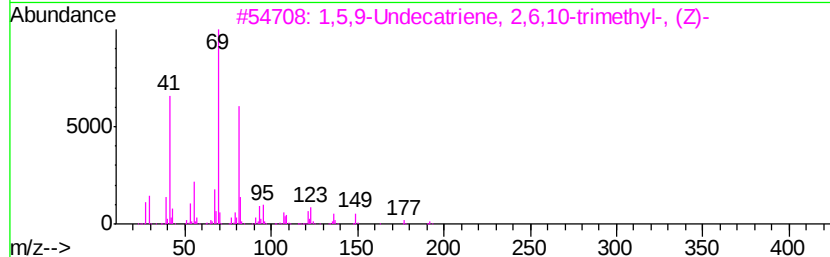
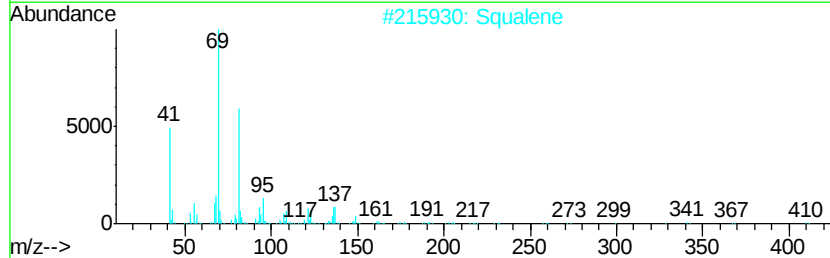
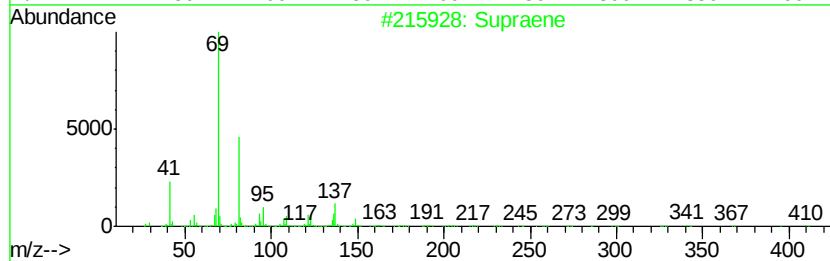
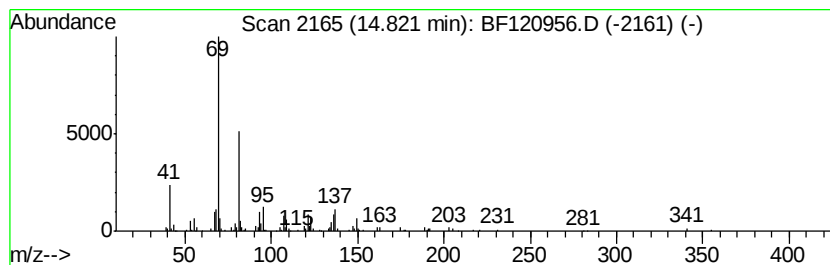
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.22 ng	145238	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072120\
Data File : BF120956.D
Acq On : 21 Jul 2020 16:14
Operator : JU/CG
Sample : L3358-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55-ST-28

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-eth...	6.65	3.0	ng	145856	1	6.82	987536	20.0
unknown8.02	8.02	3.5	ng	252394	2	8.10	1455080	20.0
Thiophane, propyl-	8.47	3.0	ng	220038	2	8.10	1455080	20.0
2,4,7,9-Tetrameth...	9.29	14.4	ng	1095480	3	9.85	1518250	20.0
unknown10.44	10.44	3.4	ng	260836	3	9.85	1518250	20.0
1-Heneicosanol	13.83	6.2	ng	469653	5	13.97	1519050	20.0
Supraene	14.82	2.2	ng	145238	6	15.42	1308520	20.0