

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
 Data File : BP000548.D
 Acq On : 07 Oct 2019 17:19
 Operator : JU
 Sample : K5213-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-1(5-10)

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_P\METHODS\8270-BP100119.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	2.334	36	42	52	rVB	56294	87147	1.54%	0.186%
2	4.469	400	405	419	rBV	1133904	1311943	23.19%	2.797%
3	4.958	484	488	496	rBV	323459	355171	6.28%	0.757%
4	5.381	556	560	571	rBV	3407055	3078544	54.42%	6.562%
5	6.399	729	733	743	rBV	4538073	4082332	72.16%	8.702%
6	6.534	752	756	759	rBV	4513608	3891973	68.80%	8.296%
7	6.763	791	795	798	rBV	1583139	1361983	24.08%	2.903%
8	6.916	817	821	824	rBV	4425129	3464769	61.25%	7.386%
9	7.316	886	889	893	rBV	2743968	2459770	43.48%	5.243%
10	8.046	1009	1013	1016	rBV	2063428	1728716	30.56%	3.685%
11	9.122	1193	1196	1200	rBV	6110782	5331807	94.25%	11.366%
12	9.522	1260	1264	1267	rBV	733568	605883	10.71%	1.292%
13	9.804	1309	1312	1316	rBV	2671515	2182300	38.58%	4.652%
14	10.599	1443	1447	1461	rBV	2744536	2379039	42.05%	5.071%
15	11.304	1563	1567	1570	rBV	2834598	2321830	41.04%	4.949%
16	11.375	1576	1579	1583	rVB2	160527	128713	2.28%	0.274%
17	12.910	1836	1840	1843	rBV	6591633	5657093	100.00%	12.059%
18	13.828	1994	1996	2004	rBV3	286458	422731	7.47%	0.901%
19	13.975	2017	2021	2028	rVB	2565860	2324722	41.09%	4.955%
20	15.451	2268	2272	2285	rVB	1919299	2539756	44.90%	5.414%
21	16.169	2391	2394	2402	rVB2	281618	513759	9.08%	1.095%
22	16.604	2464	2468	2479	rVB	375399	682188	12.06%	1.454%

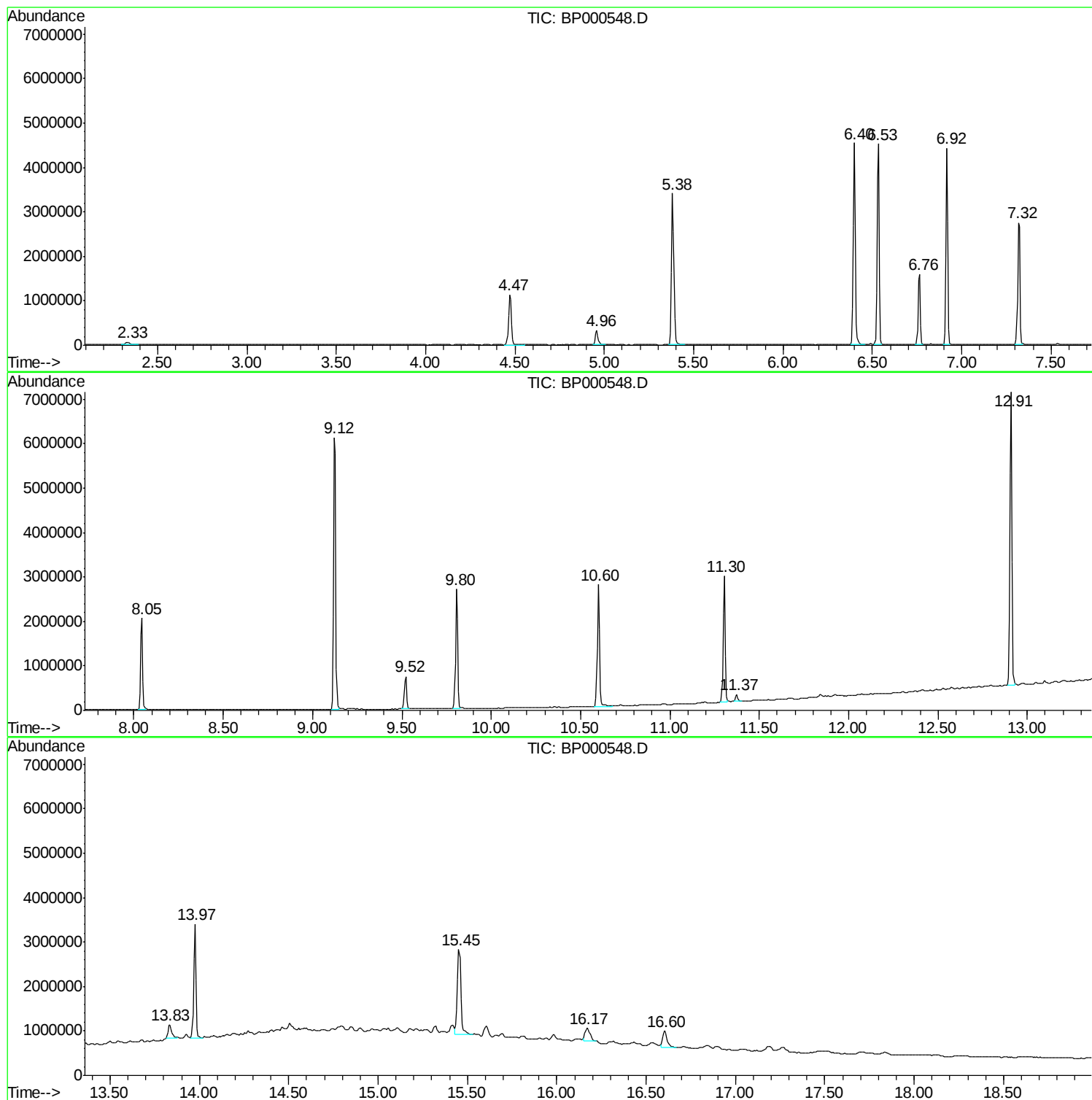
Sum of corrected areas: 46912169

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

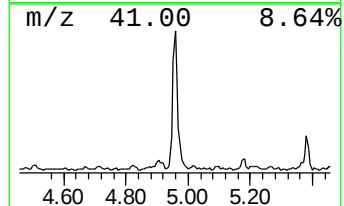
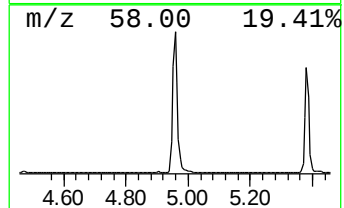
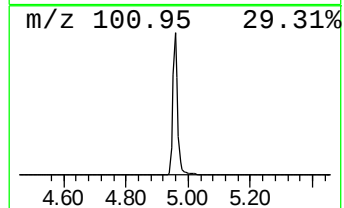
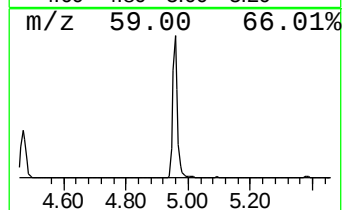
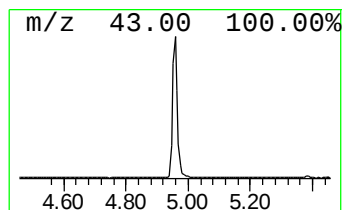
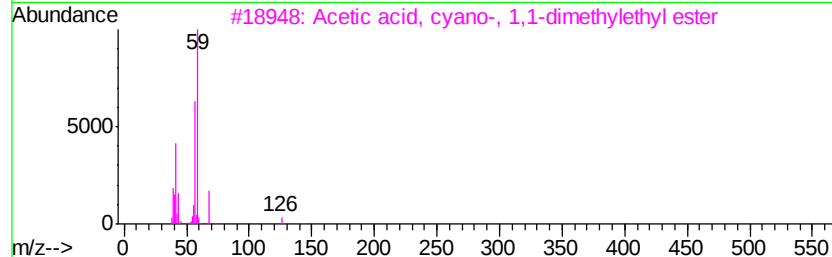
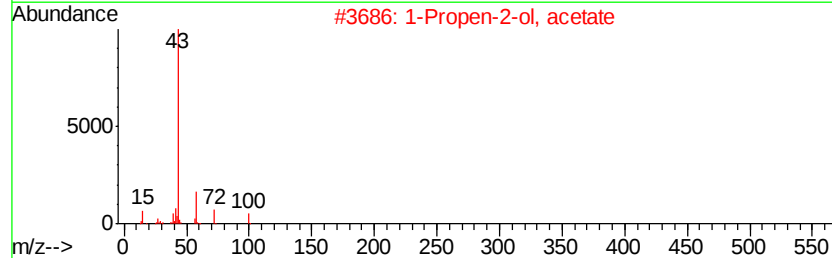
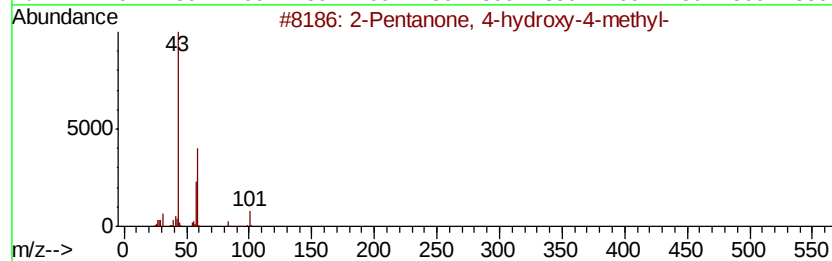
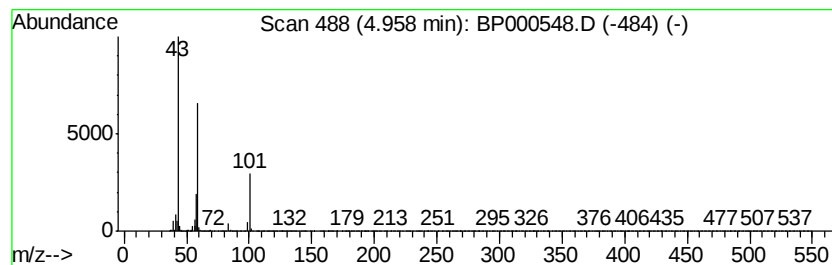
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	5.22 ng	355171	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	22
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	12
4		Acetone	58	C3H6O	000067-64-1	12
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

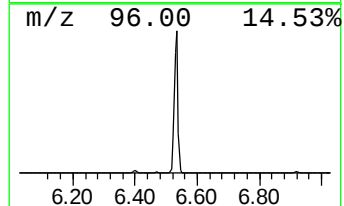
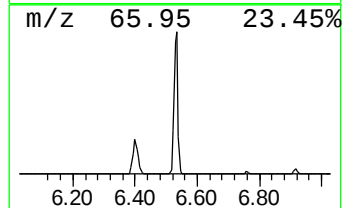
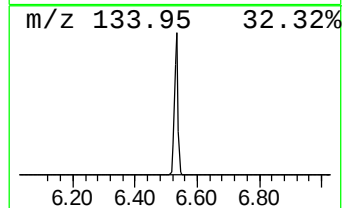
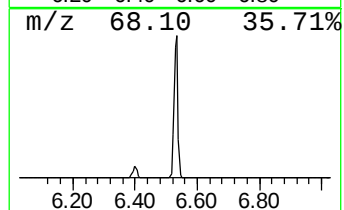
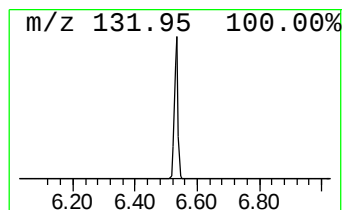
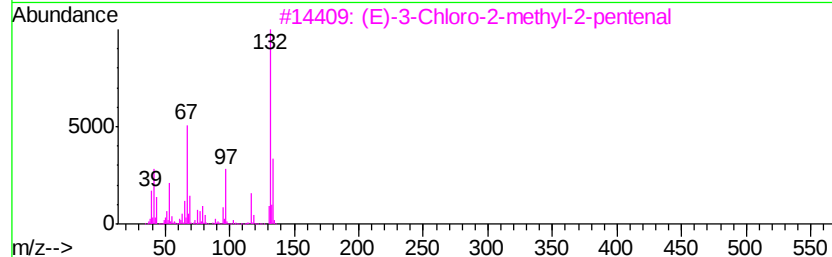
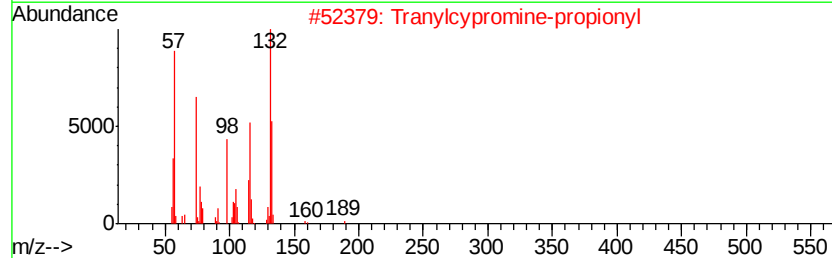
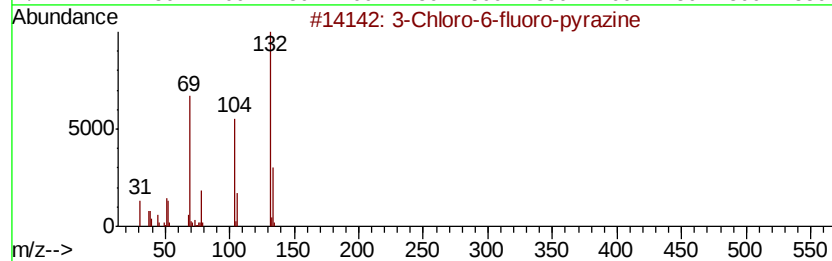
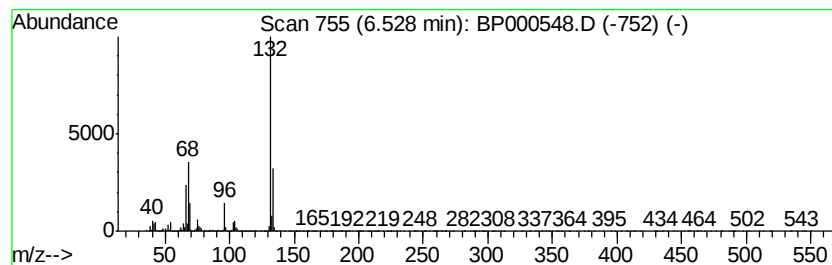
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	57.15 ng	3891970	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

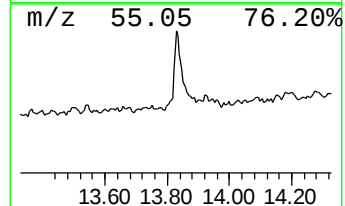
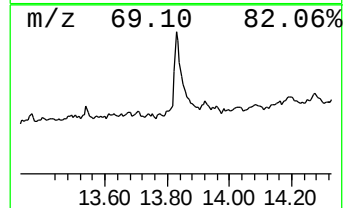
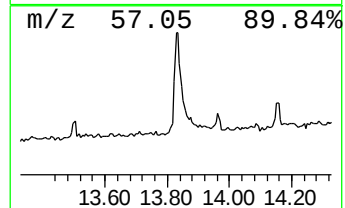
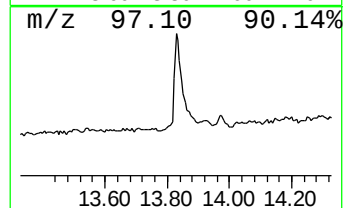
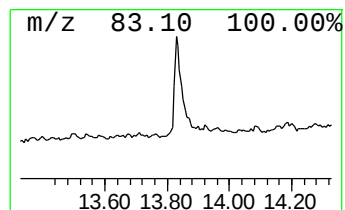
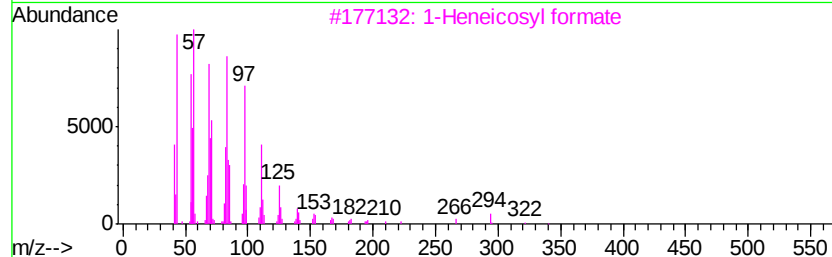
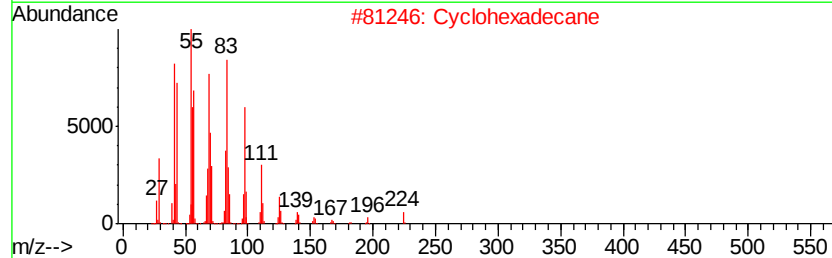
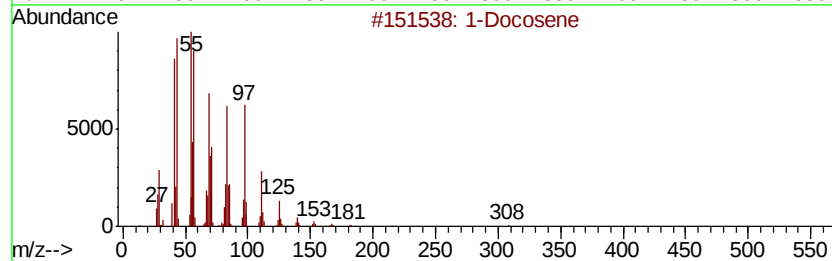
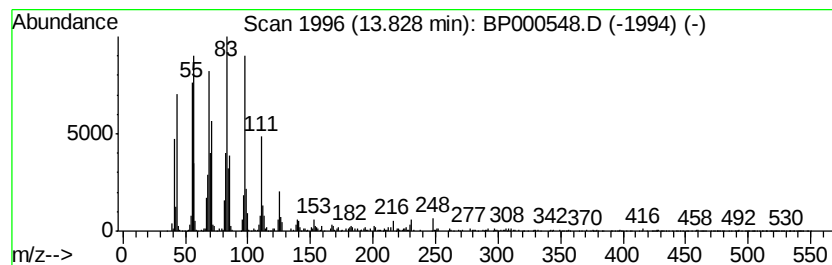
Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.83	3.64 ng	422731	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

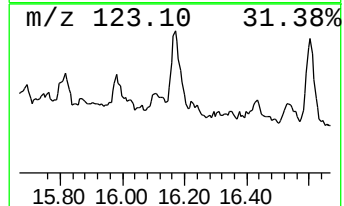
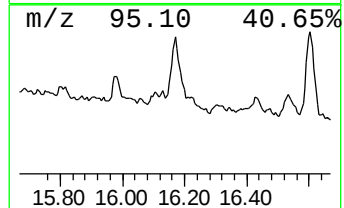
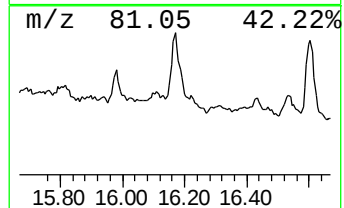
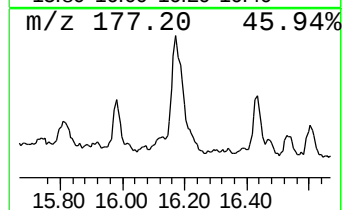
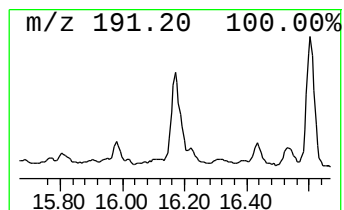
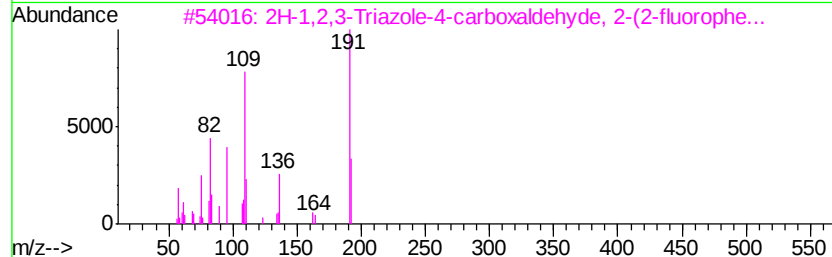
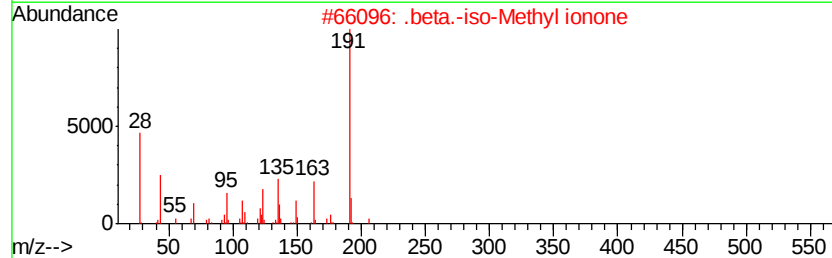
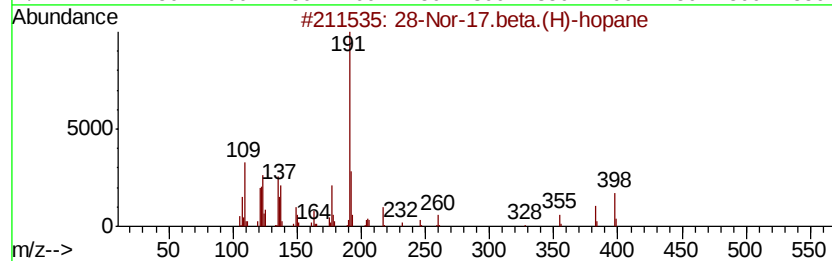
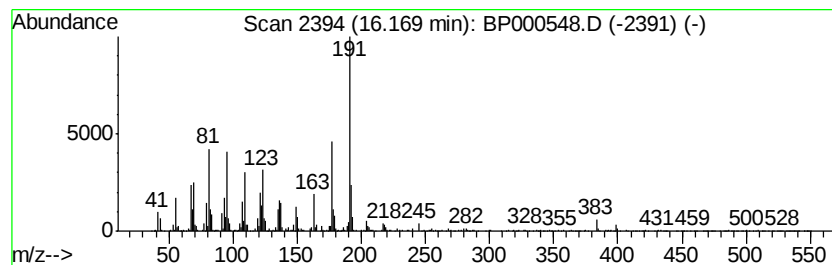
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 28-Nor-17.beta.(H)-hopane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	4.05 ng	513759	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	53
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3		2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	37
4		2-Amino-4-methyl-6-(2-thienyl)py...	191	C9H9N3S	026963-43-9	27
5		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

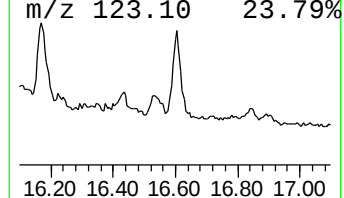
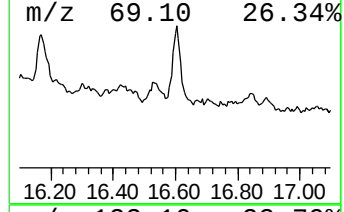
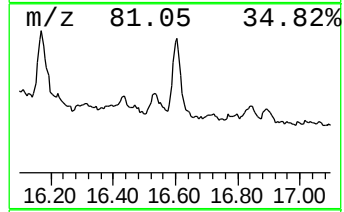
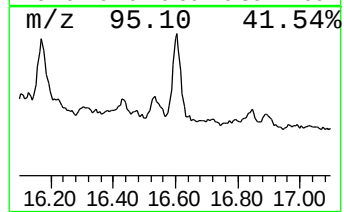
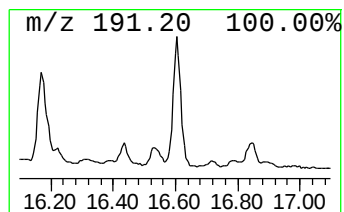
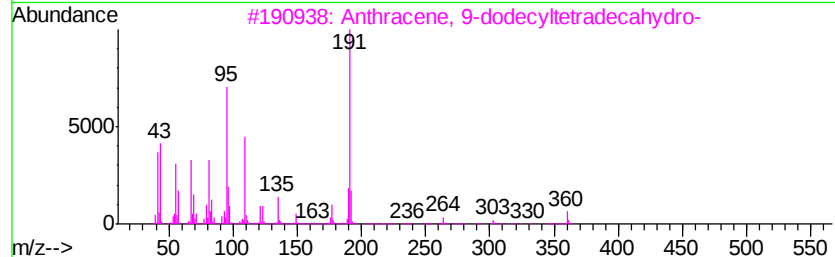
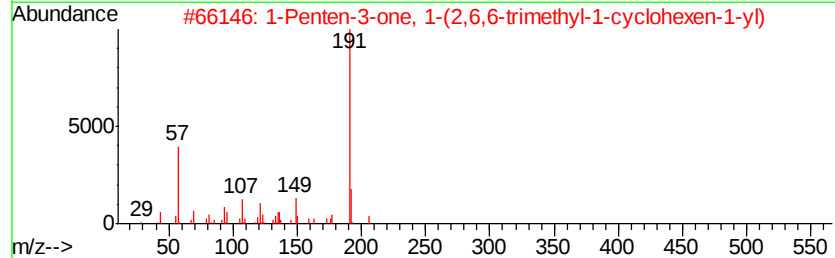
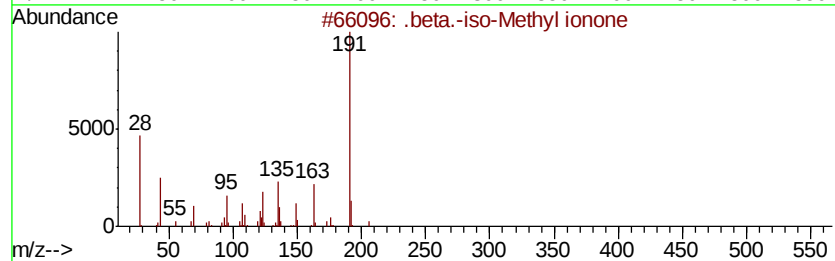
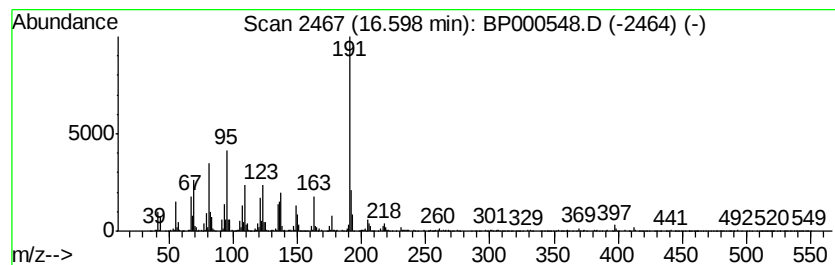
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .beta.-iso-Methyl ionone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	5.37 ng	682188	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	55
3		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	53
4		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
5		Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP100719\
Data File : BP000548.D
Acq On : 07 Oct 2019 17:19
Operator : JU
Sample : K5213-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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
2-Pentanone, 4-hy...	4.96	5.2	ng	355171	1	6.76	1361980	20.0
unknown6.53	6.53	57.1	ng	3891970	1	6.76	1361980	20.0
1-Docosene	13.83	3.6	ng	422731	5	13.97	2324720	20.0
28-Nor-17.beta.(H...	16.17	4.0	ng	513759	6	15.45	2539760	20.0
.beta.-iso-Methyl...	16.60	5.4	ng	682188	6	15.45	2539760	20.0