LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0054-051-COMP-H-ELUTRIATE

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123089.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	12	19	25	rBV	1896975	2453206	26.30%	4.035%
2	5.510	577	582	585	rBV	4487960	4230604	45.36%	6.959%
3	6.510	747	752	762	rBV2	3185961	3384499	36.28%	5.567%
4	6.716	784	787	798	rBV	269058	297588	3.19%	0.489%
5	6.892	813	817	820	rBV	1801179	1478306	15.85%	2.432%
6	7.457	905	913	916	rBV	4169052	4771354	51.15%	7.848%
7	8.175	1030	1035	1038	rBV	2272378	1943803	20.84%	3.197%
8	8.451	1078	1082	1085	rVB	110049	98742	1.06%	0.162%
9	9.257	1213	1219	1222	rBV	8087108	8265655	88.62%	13.595%
10	9.333	1228	1232	1234	rBV2	117984	113189	1.21%	0.186%
11	9.375	1234	1239	1251	rVB	1908357	2164071	23.20%	3.559%
12	9.645	1281	1285	1289	rBV	882854	733196	7.86%	1.206%
13	9.933	1330	1334	1338	rVB	2568073	2243666	24.05%	3.690%
14	10.345	1401	1404	1406	rBV2	98571	98323	1.05%	0.162%
15	10.533	1432	1436	1448	rBV3	169274	435862	4.67%	0.717%
16	10.727	1463	1469	1472	rBV	5605544	5678041	60.87%	9.339%
17	11.427	1583	1588	1591	rBV	2539808	2362676	25.33%	3.886%
18	11.957	1673	1678	1681	rBV	1066971	988233	10.59%	1.625%
19	11.986	1681	1683	1687	rVB	487541	396637	4.25%	0.652%
20	12.251	1725	1728	1732	rBV	98049	107993	1.16%	0.178%
21	12.410	1751	1755	1758	rBV	727156	599538	6.43%	0.986%
22	12.469	1762	1765	1769	rBV	195568	171253	1.84%	0.282%
23	12.510	1769	1772	1777	rBV3	82139	139302	1.49%	0.229%
24	12.674	1796	1800	1804	rVB2	87173	116173	1.25%	0.191%
25	12.739	1808	1811	1817	rBV	315813	360679	3.87%	0.593%
26	12.816	1821	1824	1826	rVB	192998	148124	1.59%	0.244%
27	13.021	1853	1859	1862	rBV	8241117	9327562	100.00%	15.342%
28	13.168	1880	1884	1888	rBV	118741	119696	1.28%	0.197%
29	13.498	1936	1940	1944	rVB	211972	207617	2.23%	0.341%
30	13.639	1960	1964	1967	rBV	833289	711843	7.63%	1.171%
31	13.674	1967	1970	1973	rVV2	224303	201633	2.16%	0.332%
32	13.716	1974	1977	1984	rVB	100865	104457	1.12%	0.172%
33	13.951	2009	2017	2033	rBV4	501084	2055724	22.04%	3.381%
34	14.074	2034	2038	2042	rVB	2353536	2066420	22.15%	3.399%
35	14.627	2124	2132	2143	rBV	32800	133218	1.43%	0.219%
36	15.210	2227	2231	2236	rVB	112640	123008	1.32%	0.202%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.562	2285	2291	2295	rBV	1302106	1600869	17.16%	2.633%
38	15.598	2295	2297	2303	rVB	102622	135437	1.45%	0.223%
39	16.051	2369	2374	2383	rVB	86286	132126	1.42%	0.217%
40	16.180	2390	2396	2399	rBV6	42642	97248	1.04%	0.160%

Sum of corrected areas: 60797571

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
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Acq On : 29 Jan 2021 18:47
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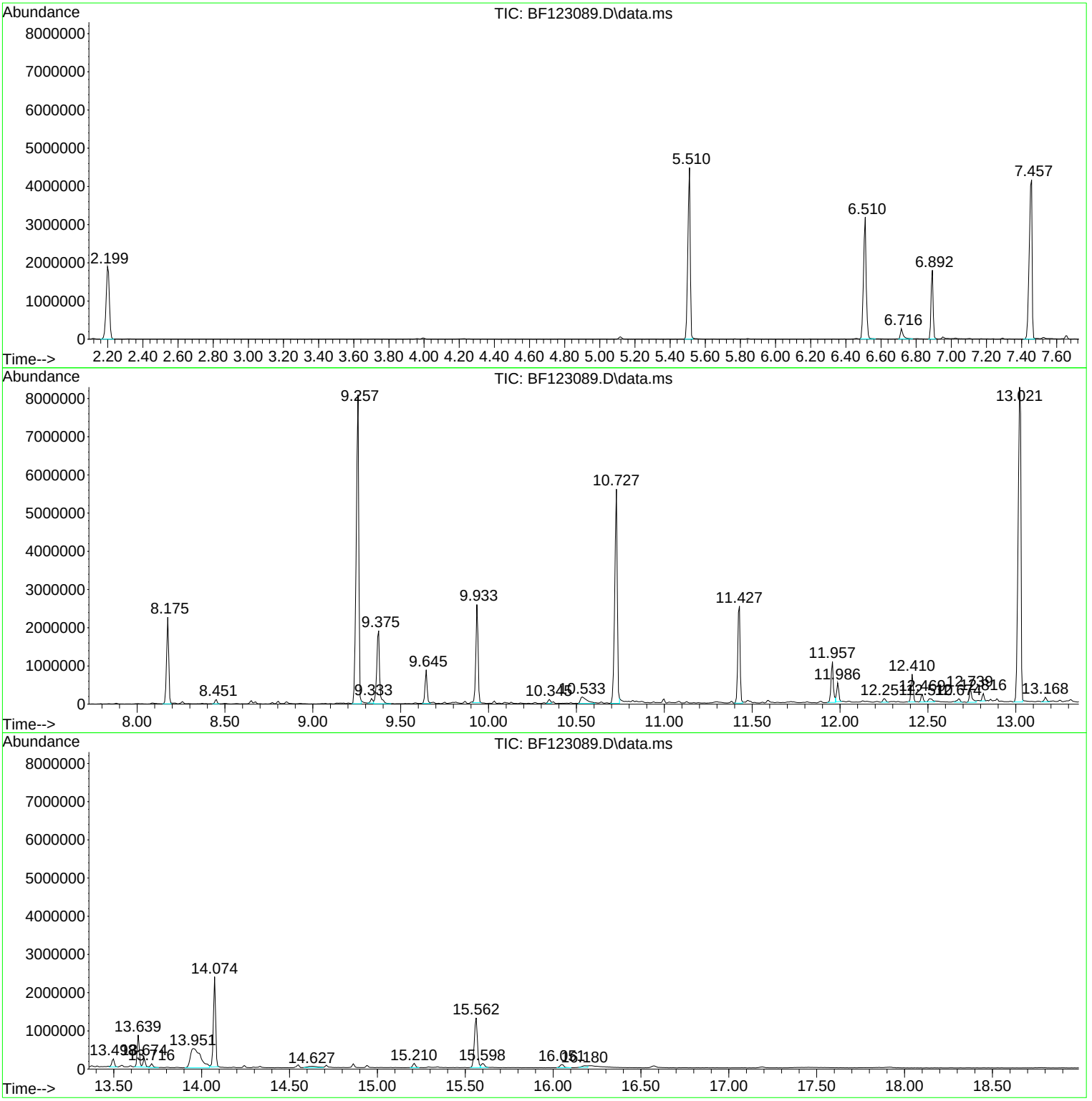
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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_F\Data\BF012921\
Data File : BF123089.D
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Operator : JU/CG
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Misc :
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Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

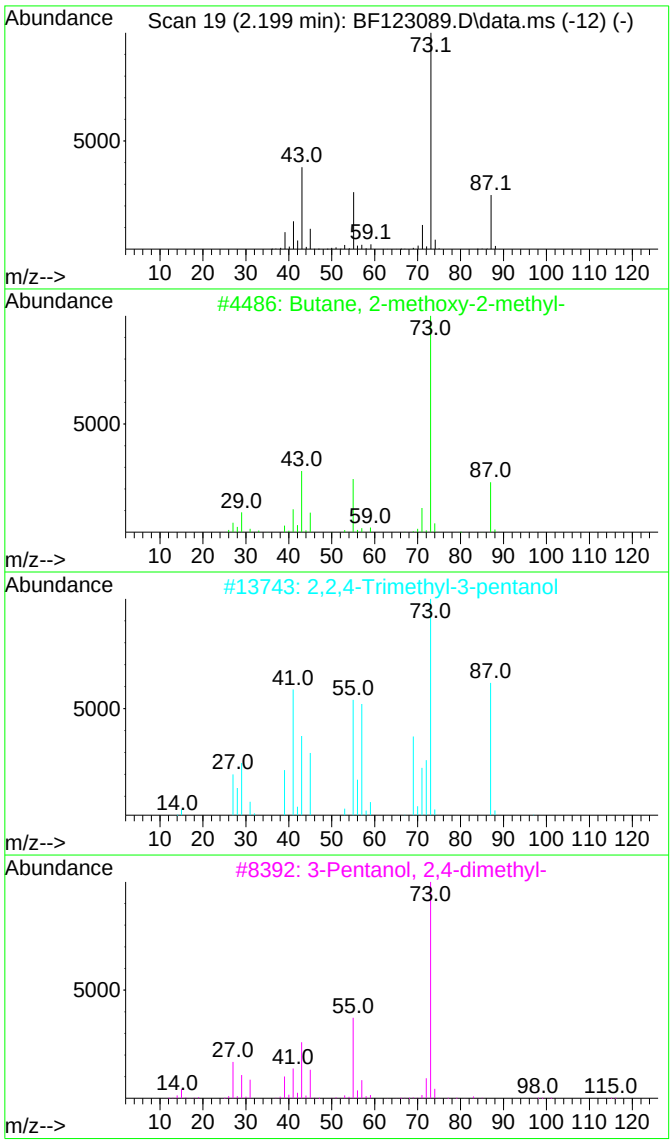
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

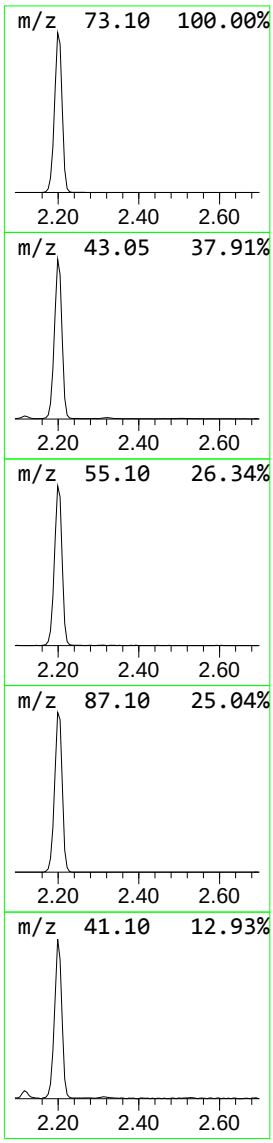
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	33.19 ng	2453210	1,4-Dichlorobenzene-d4	6.892

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

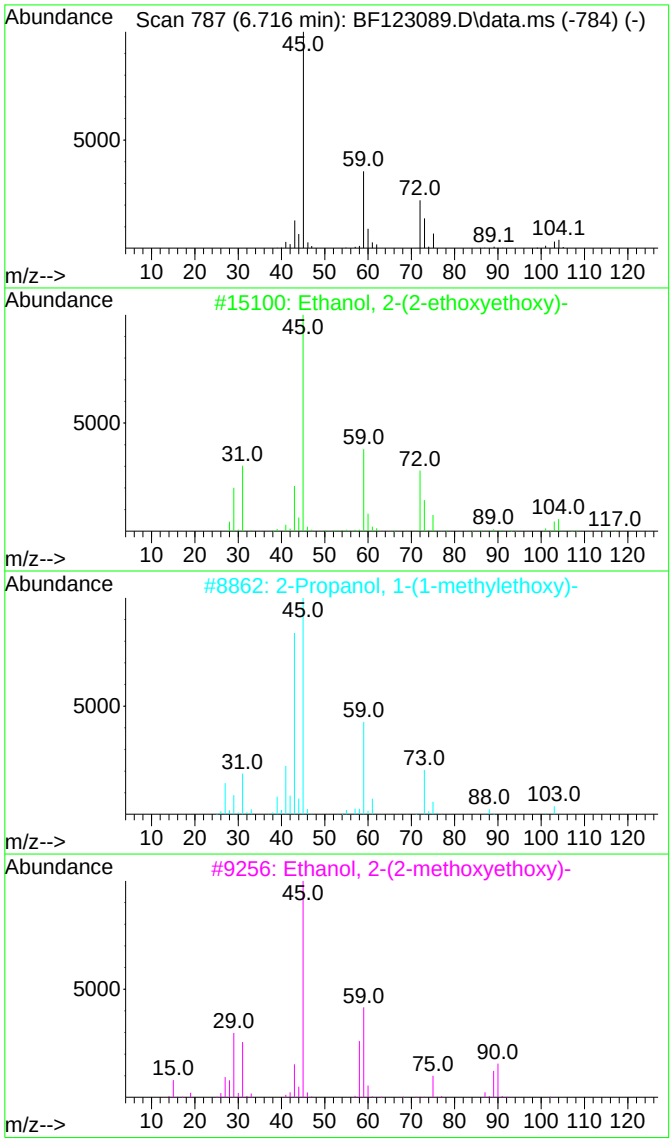
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

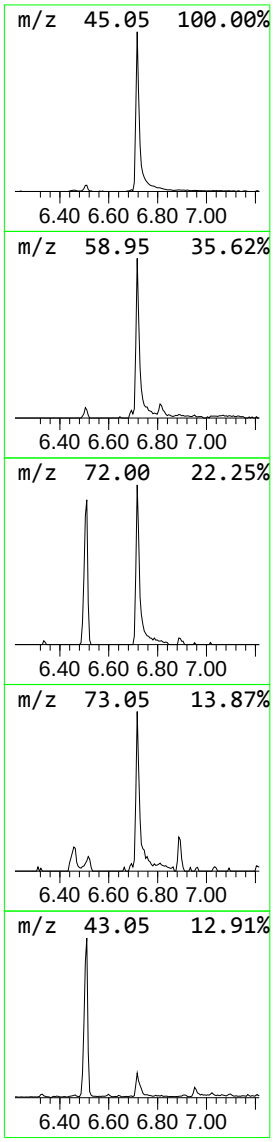
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	4.03 ng	297588	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

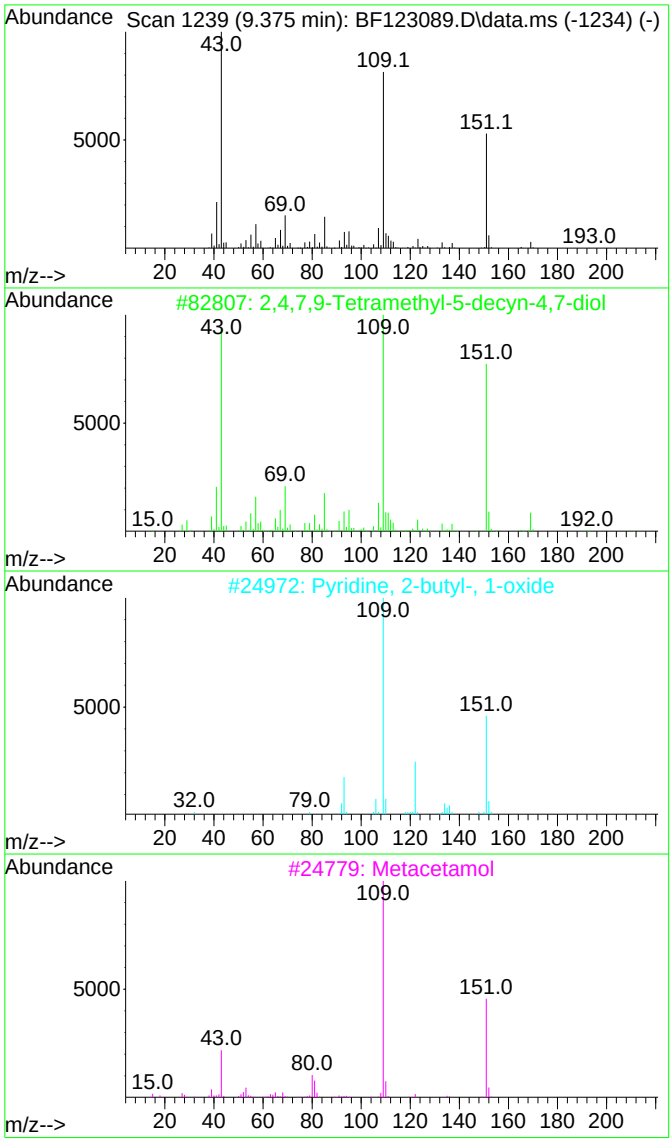
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

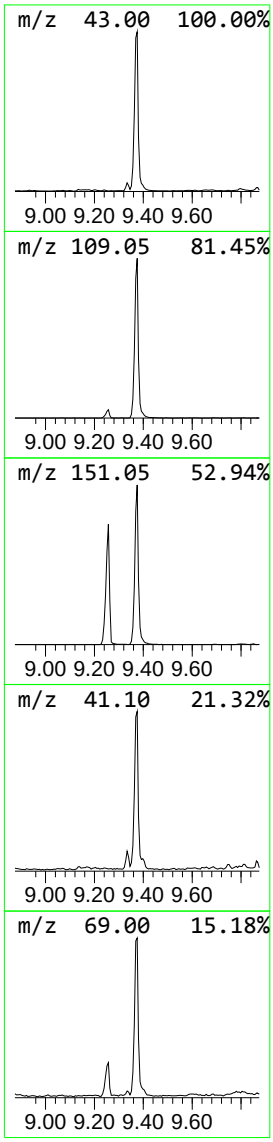
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.375	19.29 ng	2164070	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	59
4	1-(1,2,3-Trimethyl-cyclopent-2-e...	152	C10H16O	070987-81-4	43
5	3,6-Dimethyl-6-hepten-4-yn-3-ol	138	C9H14O	003601-67-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

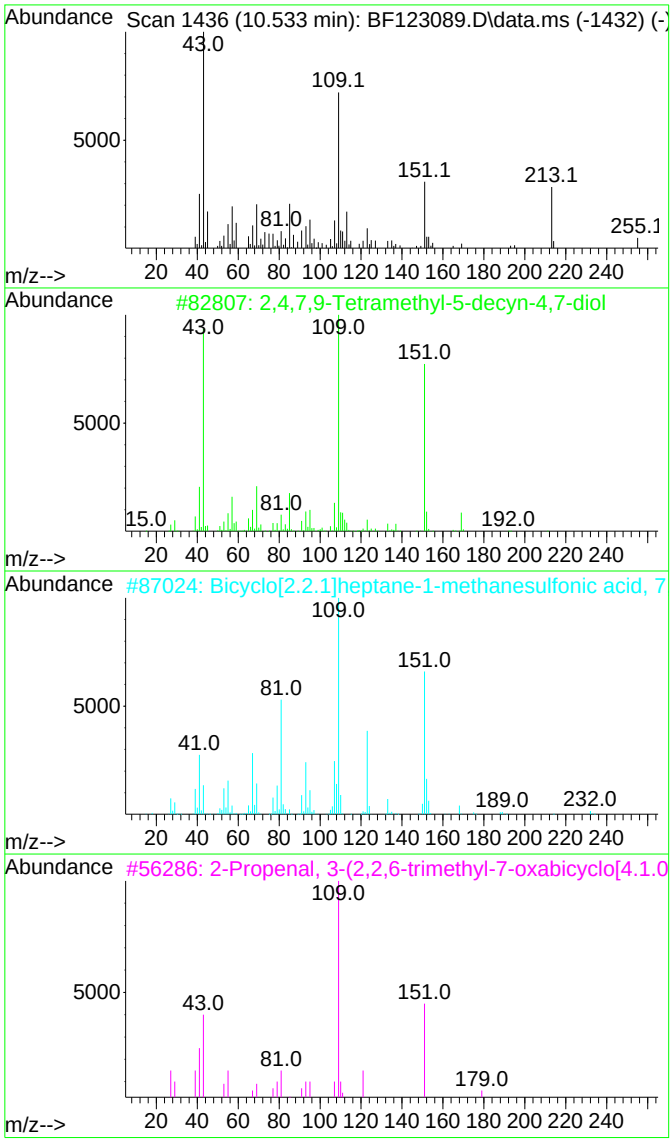
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

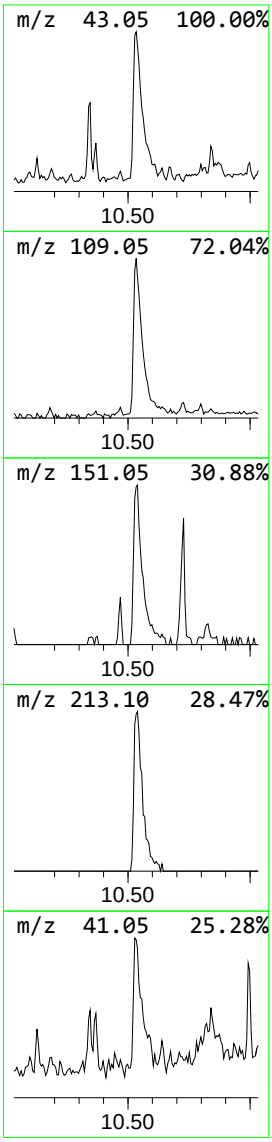
****

Peak Number 4 unknown10.533 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	3.89 ng	435862	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53
2	Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	35
3	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	32
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	27
5	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	25





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Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

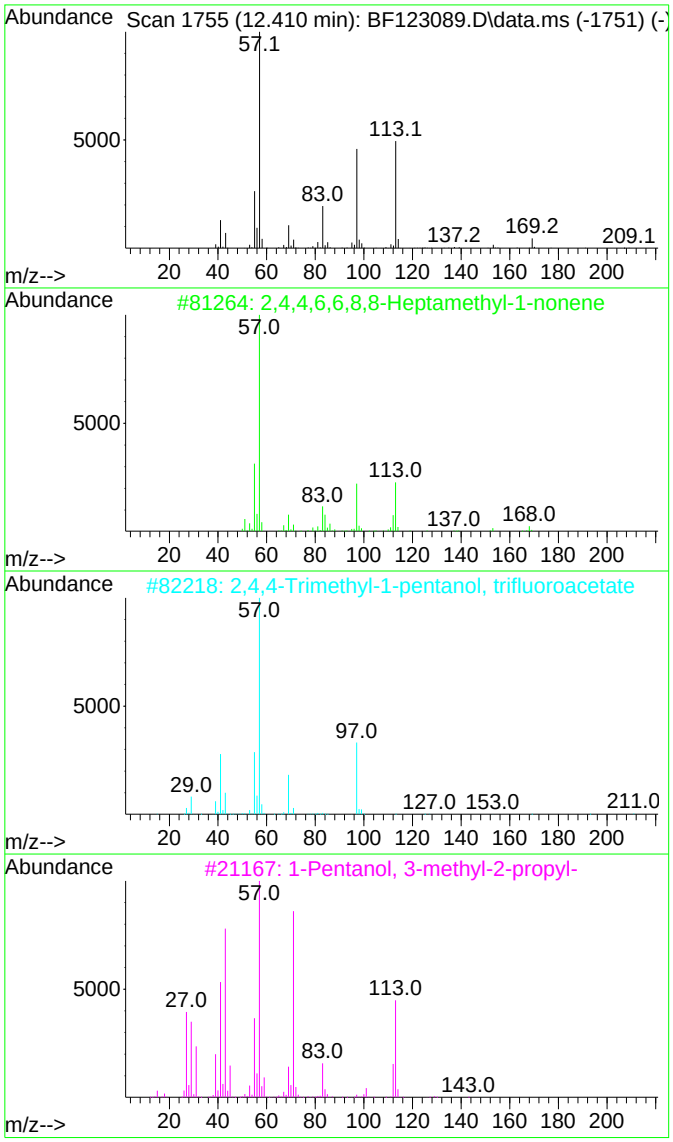
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

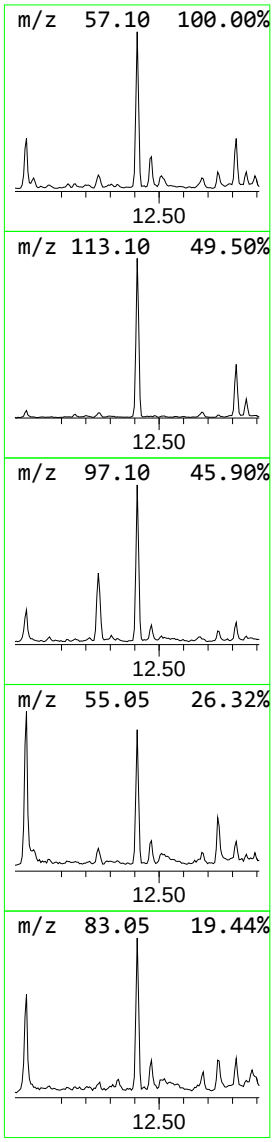
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown12.410 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	5.08 ng	599538	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	45
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	35
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	25
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	12





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ALS Vial : 18 Sample Multiplier: 1

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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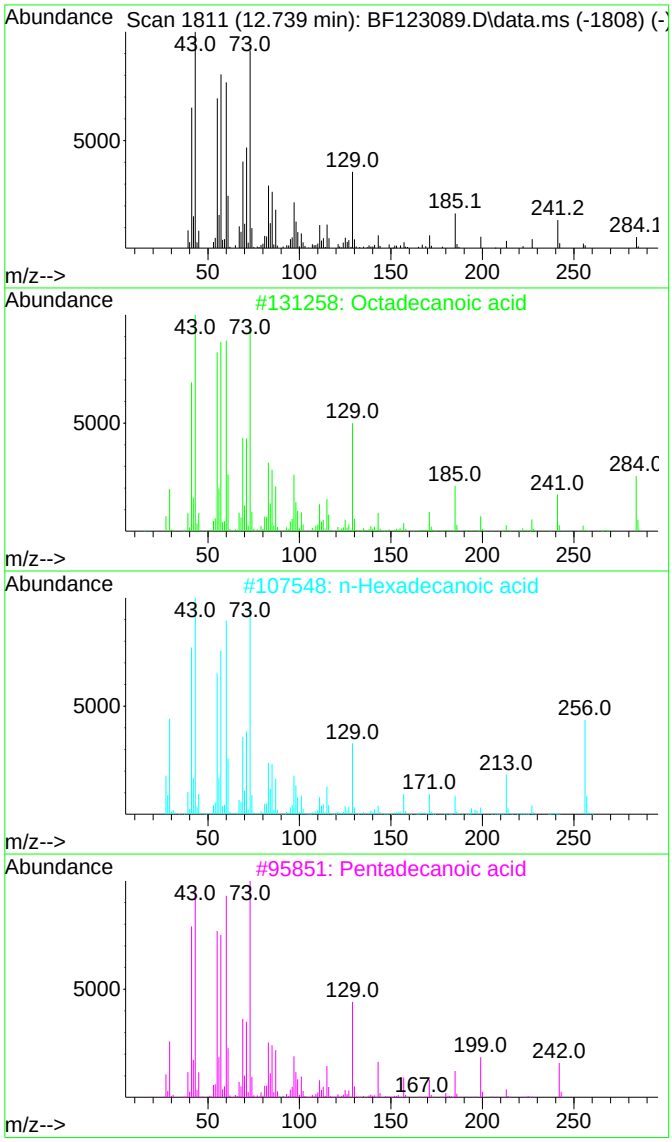
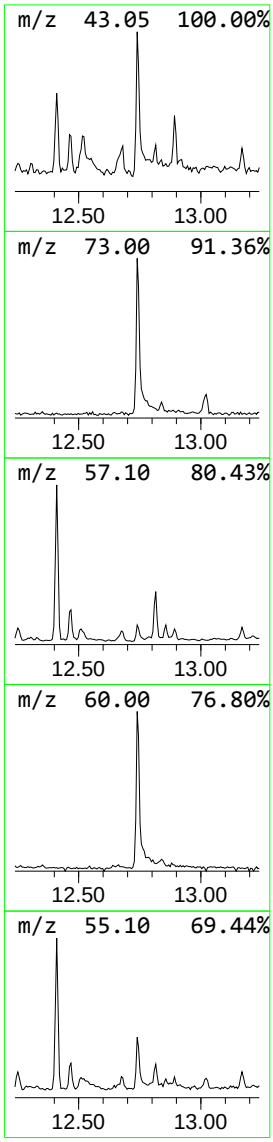
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	3.05 ng	360679	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Instrument :
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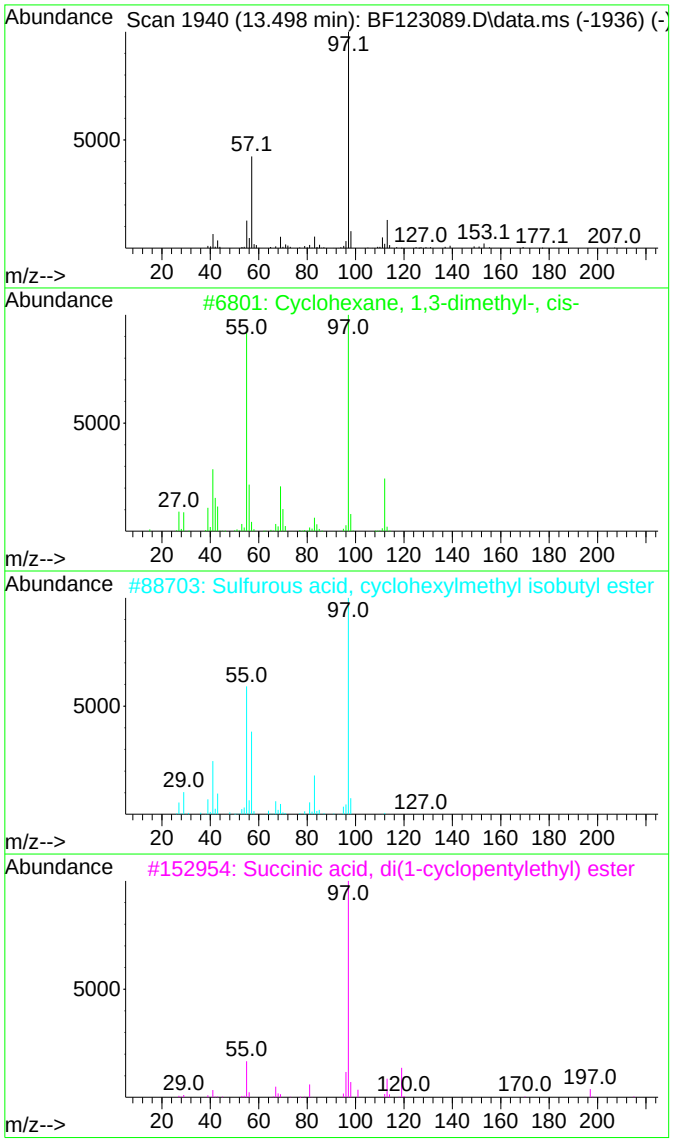
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

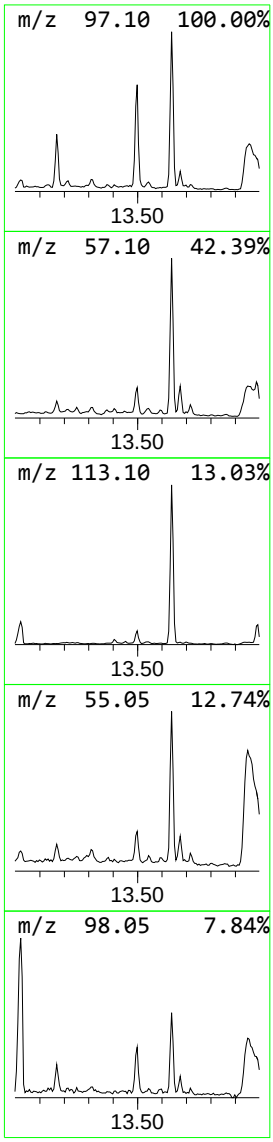
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	2.01 ng	207617	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
2	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	45
3	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	39
4	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	39
5	2-Thiopheneacetic acid, butyl ester	198	C10H14O2S	060639-72-7	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

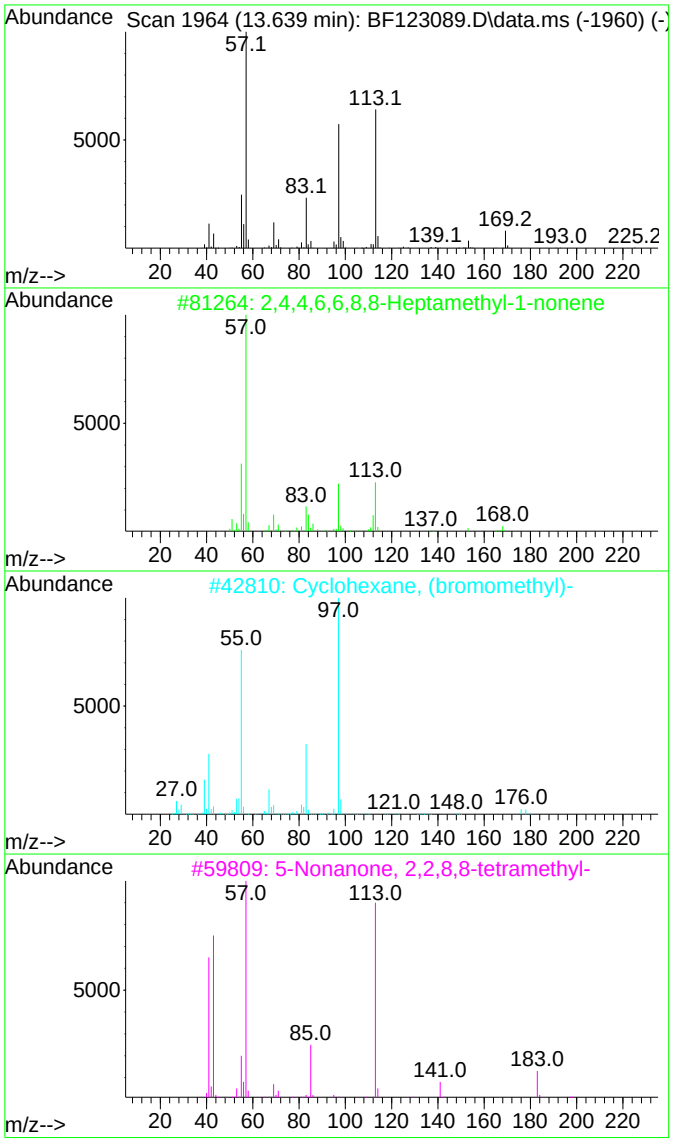
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

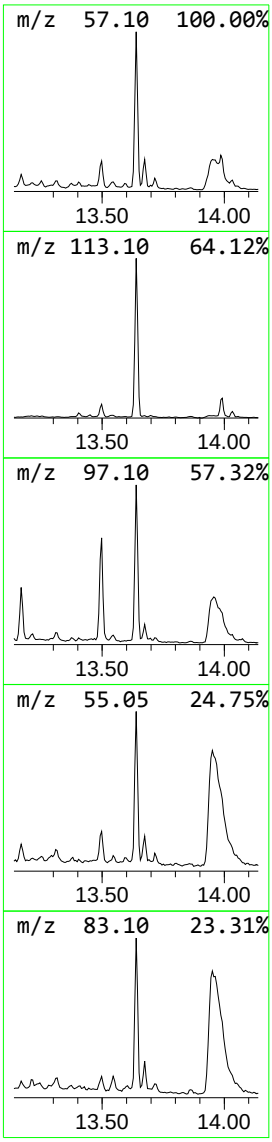
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	6.89 ng	711843	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	83
2	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	35
3	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	25
4	Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	22
5	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0054-051-COMP-H-ELUTRIATE

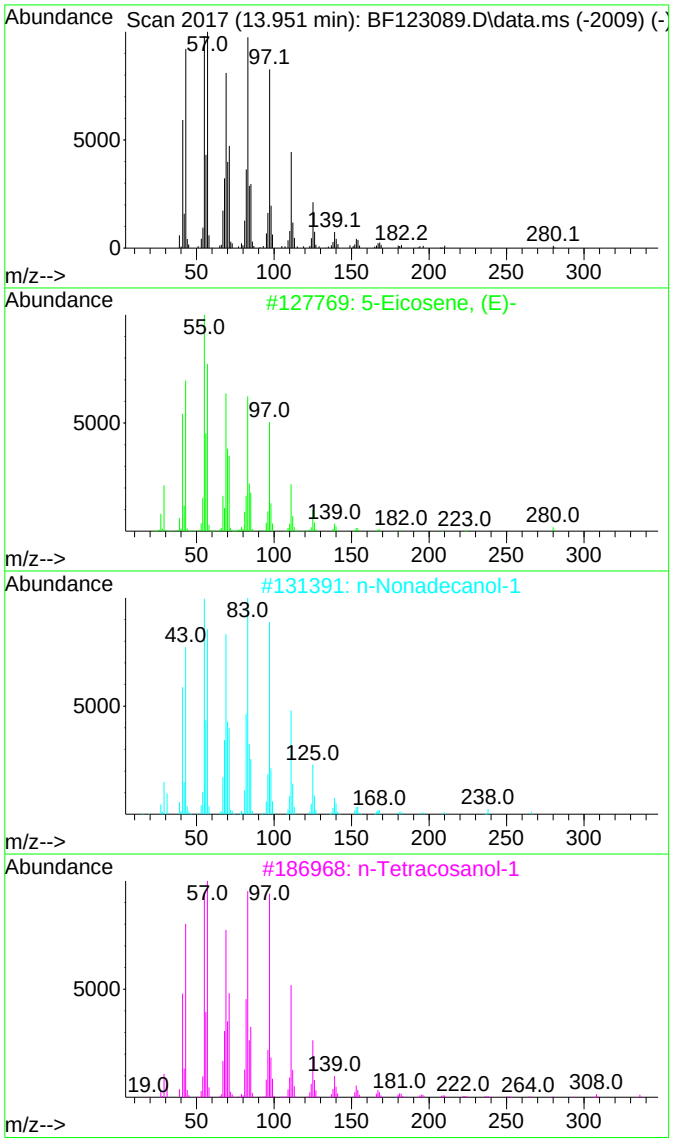
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

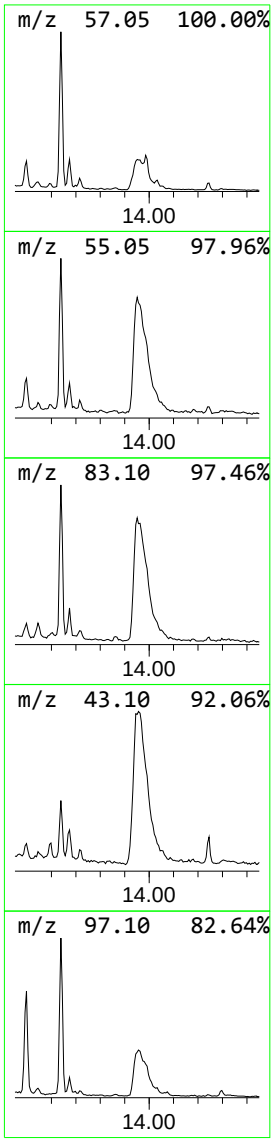
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	19.90 ng	2055720	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123089.D
Acq On : 29 Jan 2021 18:47
Operator : JU/CG
Sample : M1263-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0054-051-COMP-H-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.199	33.2	ng	2453210	1	6.892	1478310	20.0
Ethanol, 2-(2-e...	6.716	4.0	ng	297588	1	6.892	1478310	20.0
2,4,7,9-Tetrame...	9.375	19.3	ng	2164070	3	9.933	2243670	20.0
unknown10.533	10.533	3.9	ng	435862	3	9.933	2243670	20.0
unknown12.410	12.410	5.1	ng	599538	4	11.427	2362680	20.0
Octadecanoic acid	12.739	3.0	ng	360679	4	11.427	2362680	20.0
Cyclohexane, 1,...	13.498	2.0	ng	207617	5	14.074	2066420	20.0
2,4,4,6,6,8,8-H...	13.639	6.9	ng	711843	5	14.074	2066420	20.0
5-Eicosene, (E)-	13.951	19.9	ng	2055720	5	14.074	2066420	20.0