LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-A

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122402.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	21	rVB	499162	701241	1.13%	0.668%
2	3.575	243	253	262	rBV	1328731	2264315	3.66%	2.157%
3	4.557	396	420	422	rBV	11958671	61869416	100.00%	58.932%
4	5.104	502	513	516	rBV	4717248	8600145	13.90%	8.192%
5	6.863	808	812	815	rBV	1548649	1199868	1.94%	1.143%
6	7.181	862	866	870	rBV	1824084	1670520	2.70%	1.591%
7	7.428	903	908	911	rBV	2663513	2657546	4.30%	2.531%
8	7.551	925	929	937	rVB	923307	738165	1.19%	0.703%
9	7.681	947	951	954	rBV	1068291	869234	1.40%	0.828%
10	8.151	1027	1031	1034	rBV	1824663	1553011	2.51%	1.479%
11	9.228	1209	1214	1217	rBV	5820182	5100251	8.24%	4.858%
12	9.910	1325	1330	1333	rBV	2181237	1906582	3.08%	1.816%
13	11.398	1578	1583	1586	rBV	2249074	2019876	3.26%	1.924%
14	12.716	1802	1807	1821	rBV	690356	1068278	1.73%	1.018%
15	12.992	1849	1854	1857	rBV	6182661	6207300	10.03%	5.913%
16	13.898	2004	2008	2022	rBV	578421	1150671	1.86%	1.096%
17	14.039	2028	2032	2036	rBV	2411721	2266754	3.66%	2.159%
18	15.174	2222	2225	2238	rVB2	313227	801795	1.30%	0.764%
19	15.521	2278	2284	2288	rBV	1897778	2339794	3.78%	2.229%

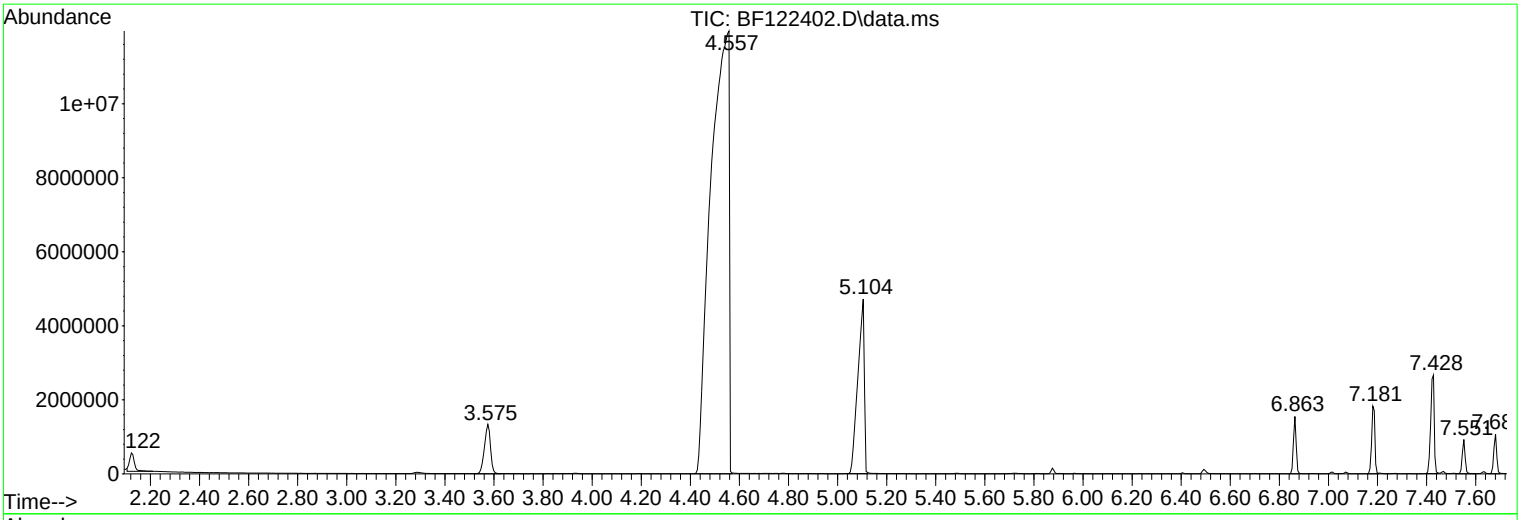
Sum of corrected areas: 104984762

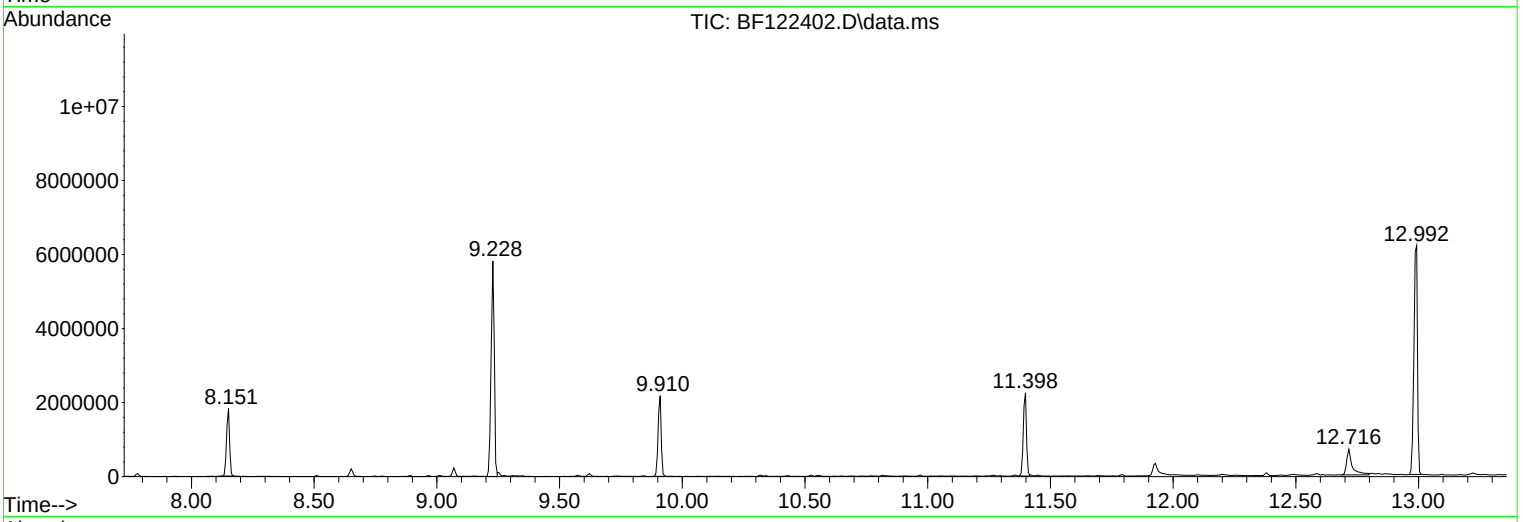
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

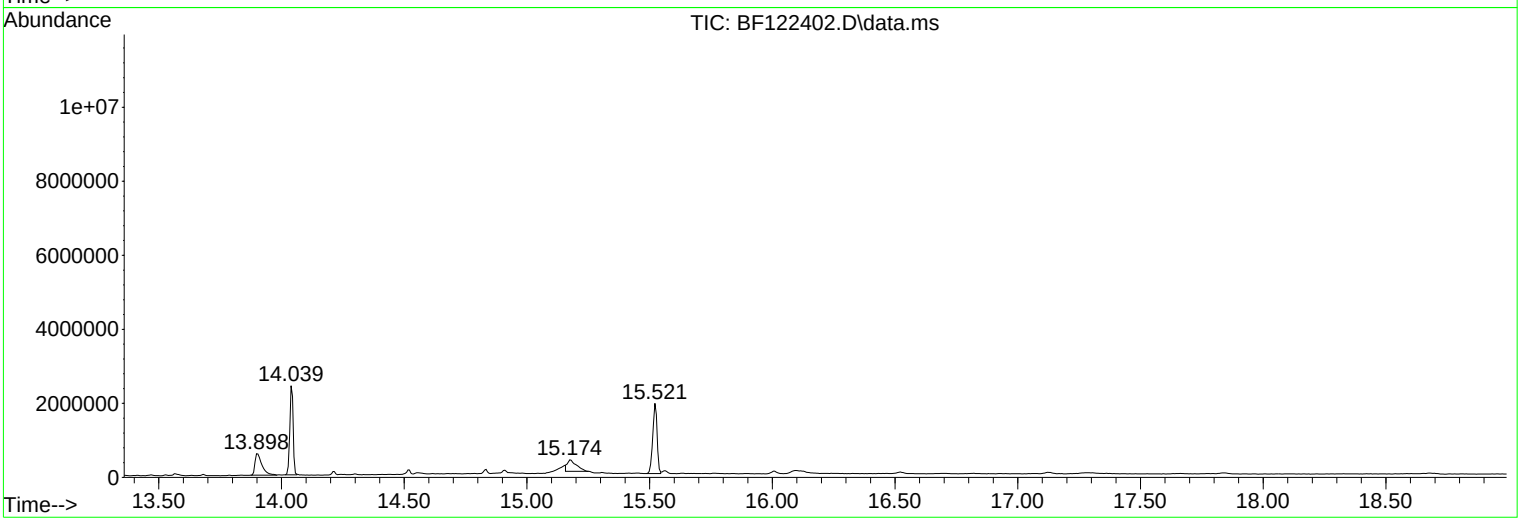
Instrument :
BNA_F
ClientSampleId :
MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-A

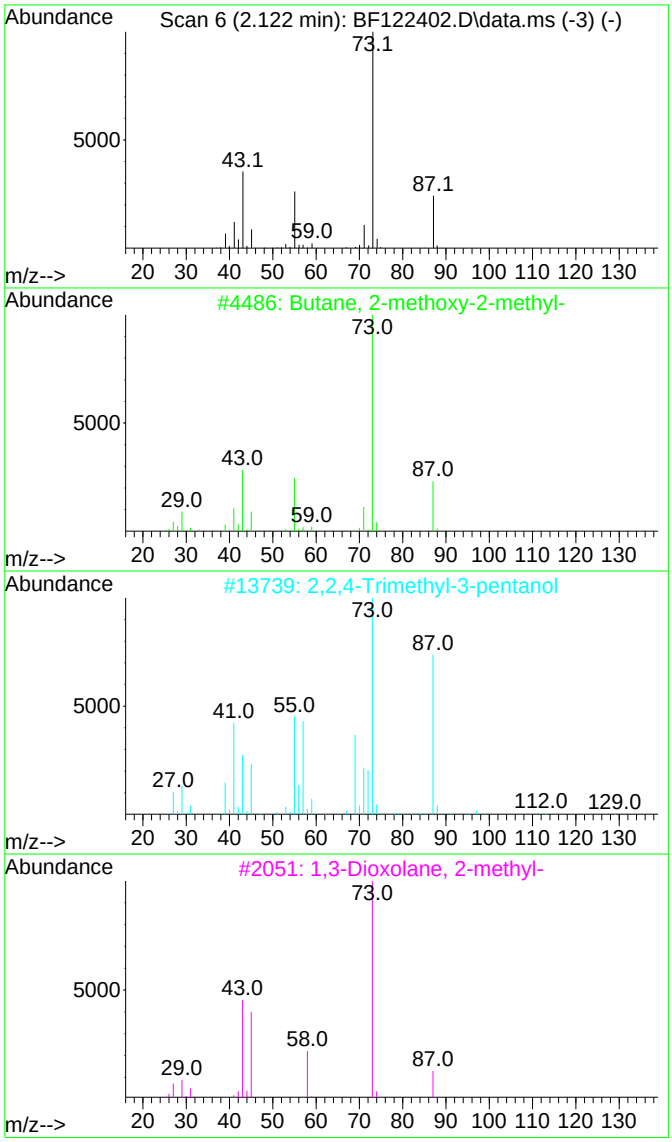
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

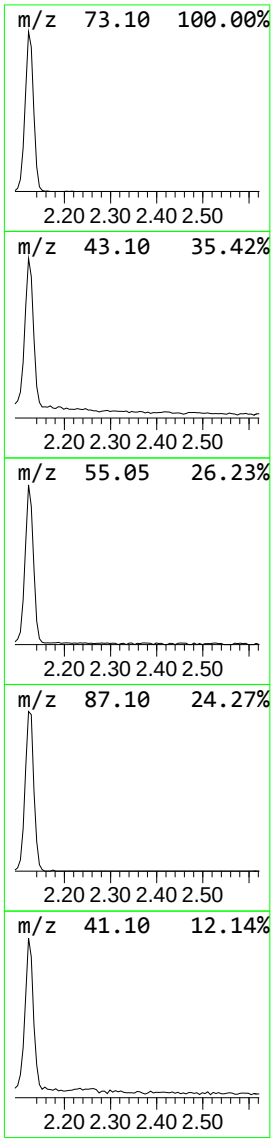
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	11.69 ng	701241	1,4-Dichlorobenzene-d4	6.863

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

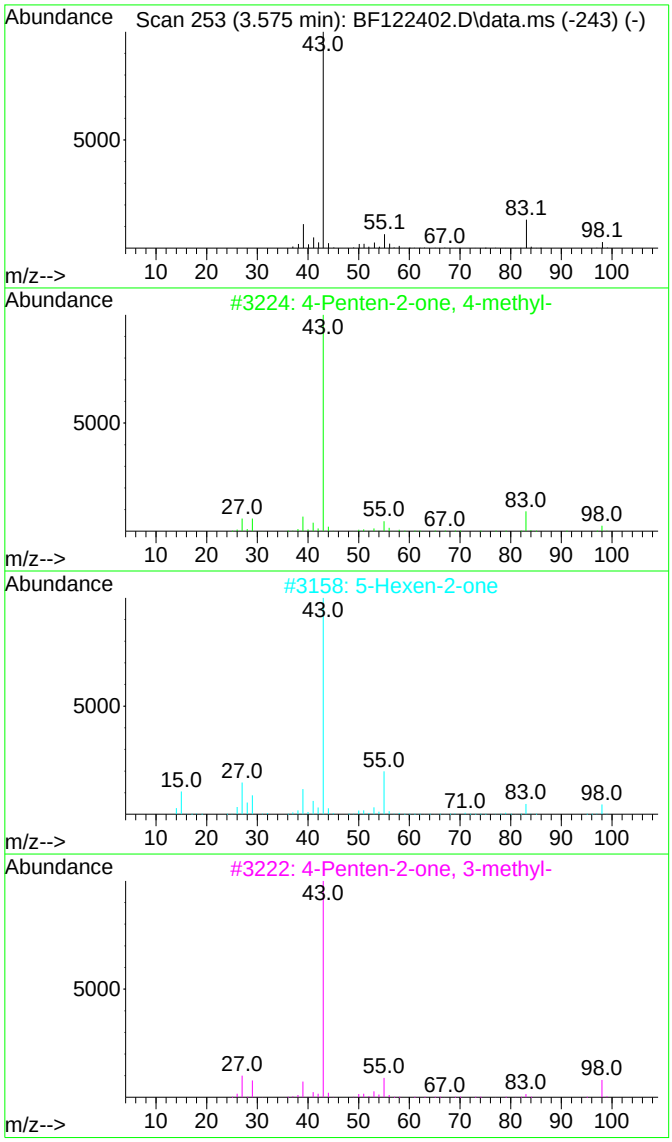
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

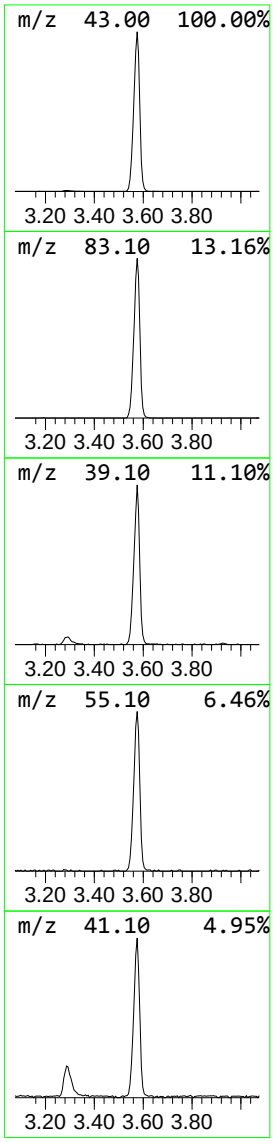
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.575	37.74 ng	2264320	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	50
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	28
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

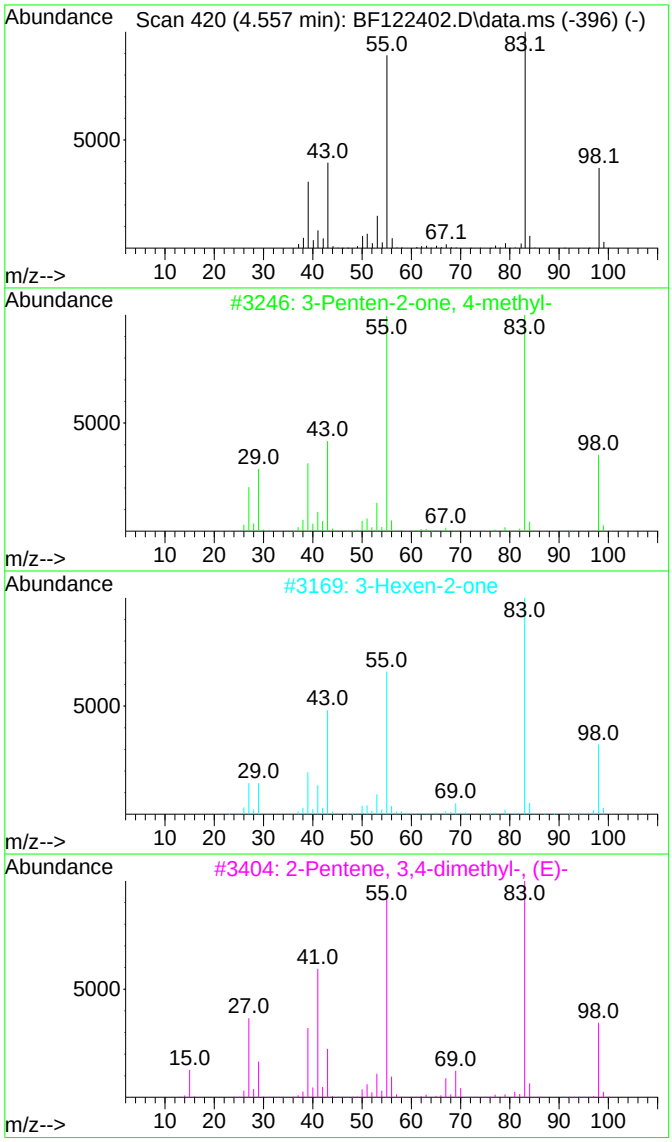
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

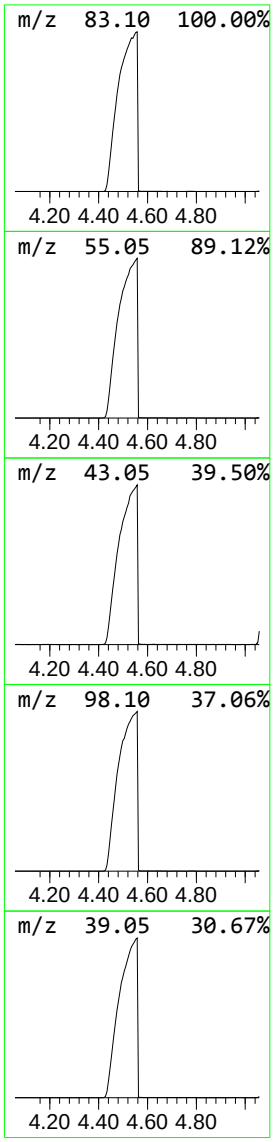
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	1031.27 ng	61869400	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

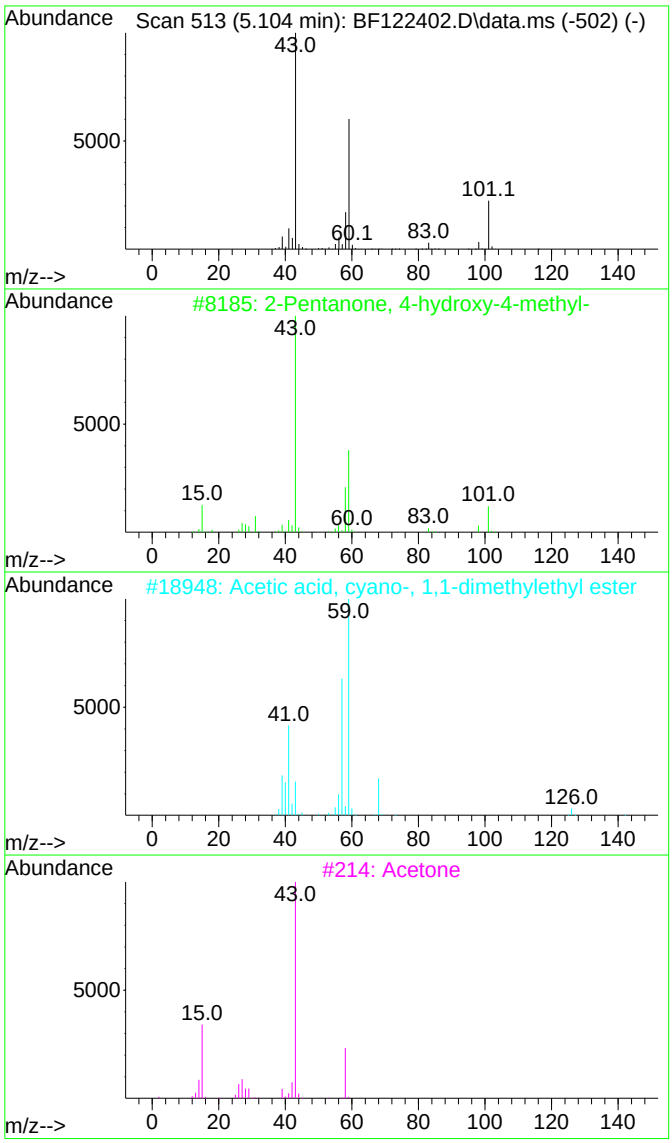
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

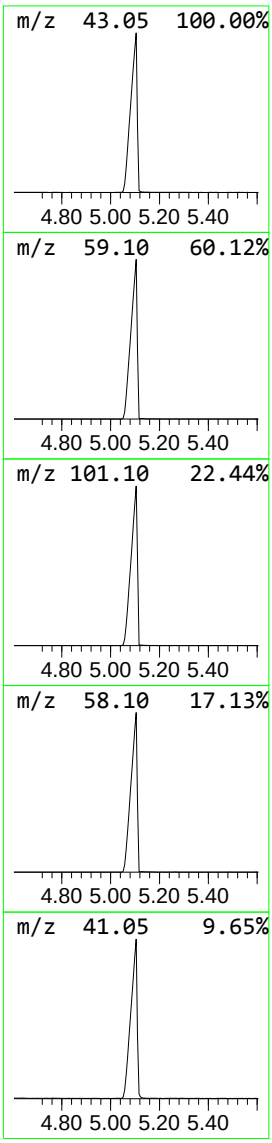
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	143.35 ng	8600150	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

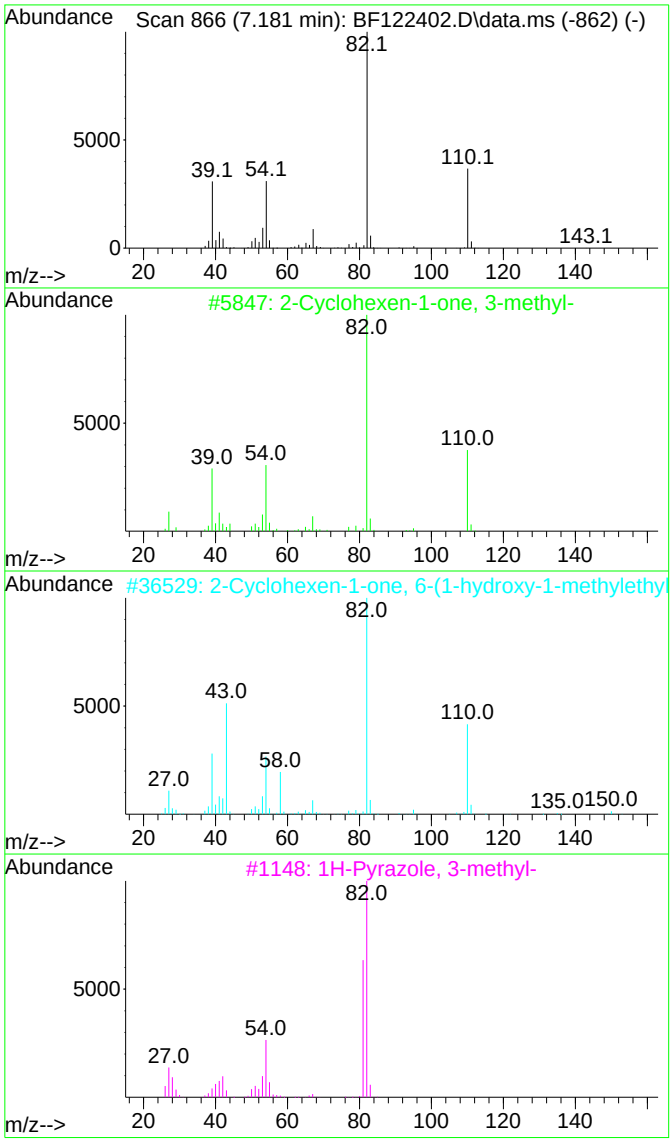
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

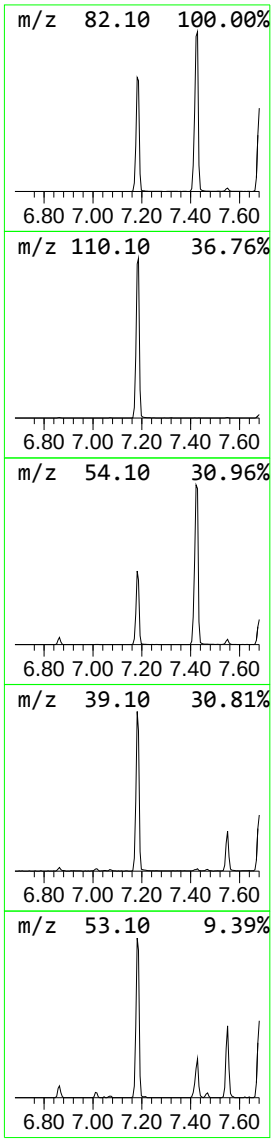
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	27.85 ng	1670520	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	50
5	Azeleonitrile	150	C9H14N2	001675-69-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

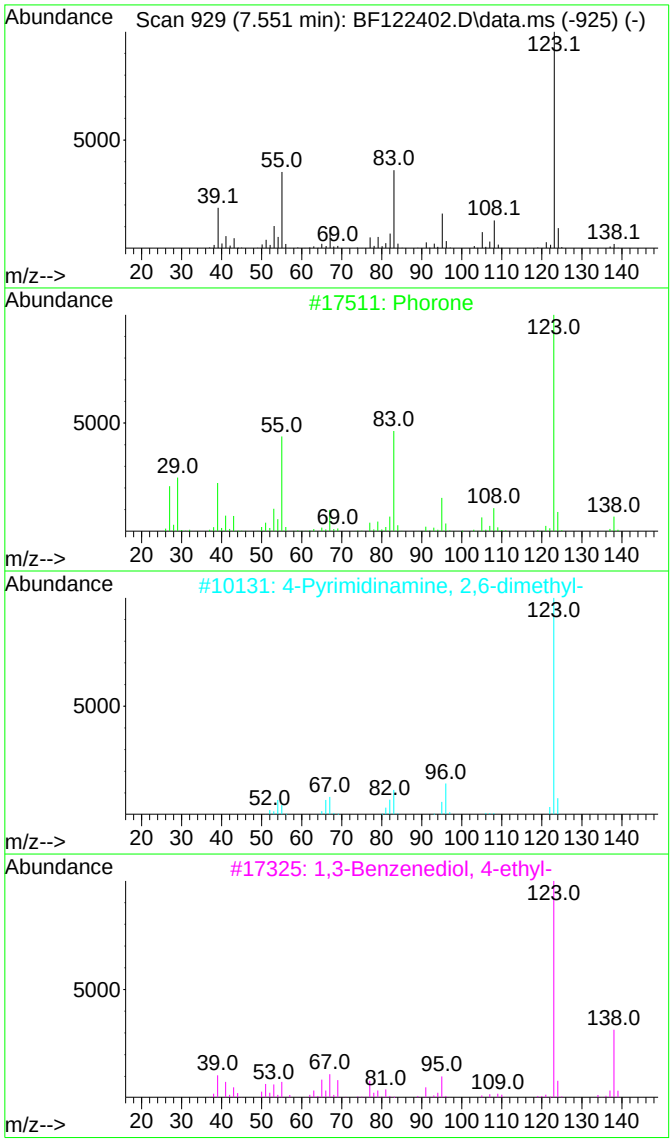
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

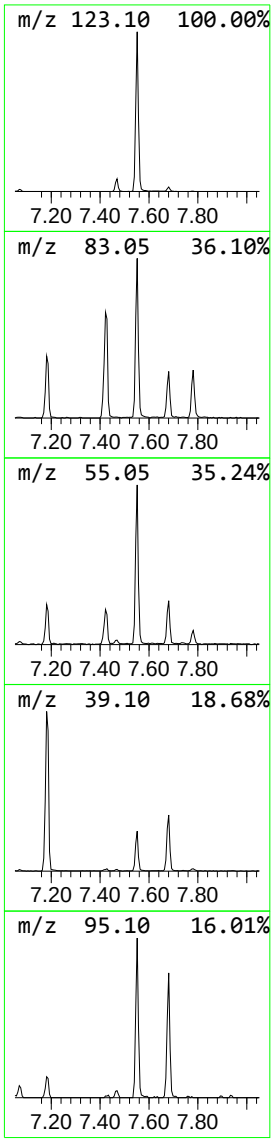
****

Peak Number 6 Phorone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.551	9.51 ng	738165	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phorone	138	C9H14O	000504-20-1	90
2	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	53
3	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	53
4	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	53
5	4-Fluorobenzoic acid, 2-isopropo...	274	C16H15FO3	1000299-05-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

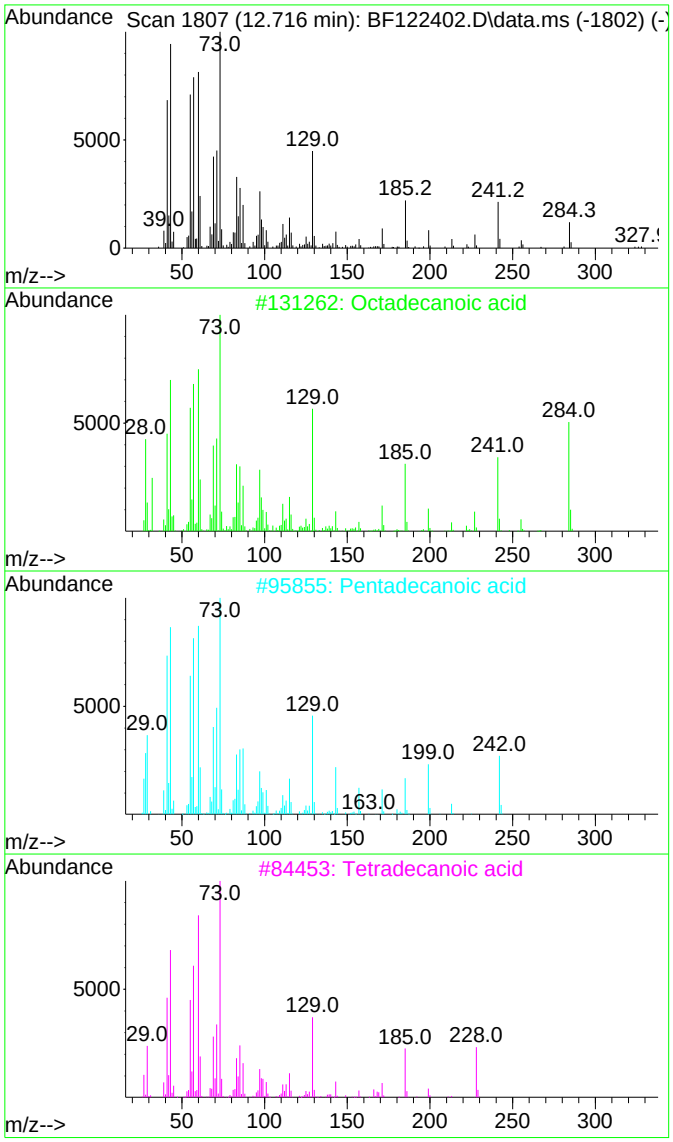
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

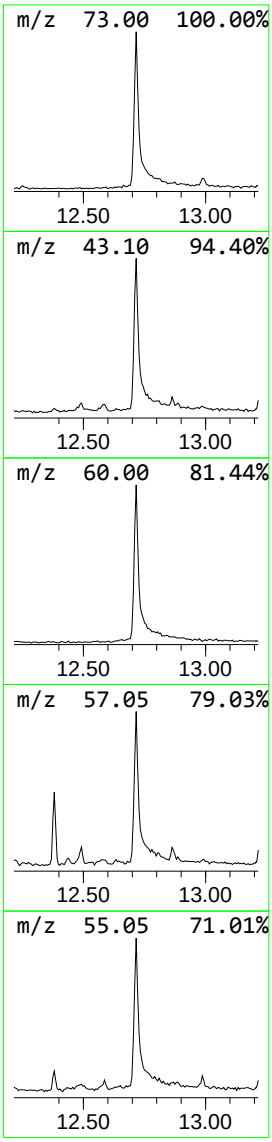
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	10.58 ng	1068280	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

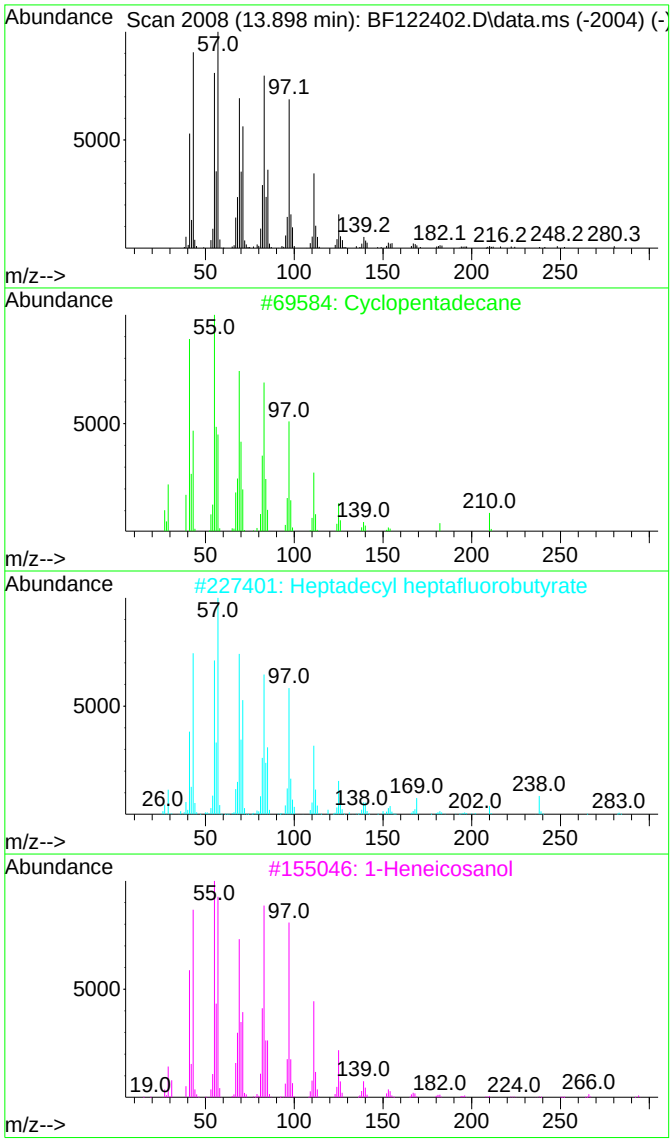
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

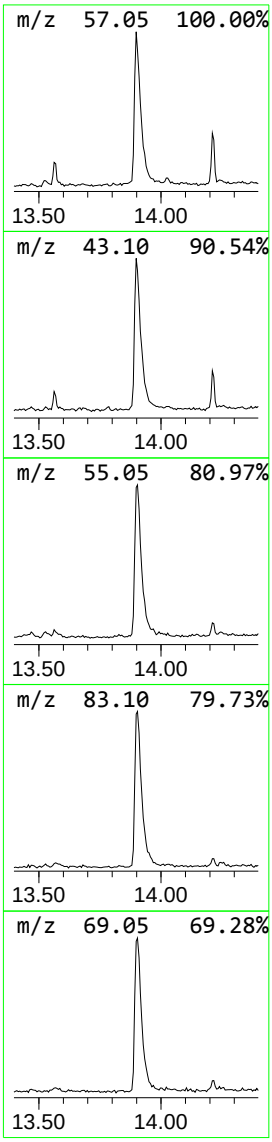
****

Peak Number 8 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	10.15 ng	1150670	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Cyclotridecane	182	C13H26	000295-02-3	92
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

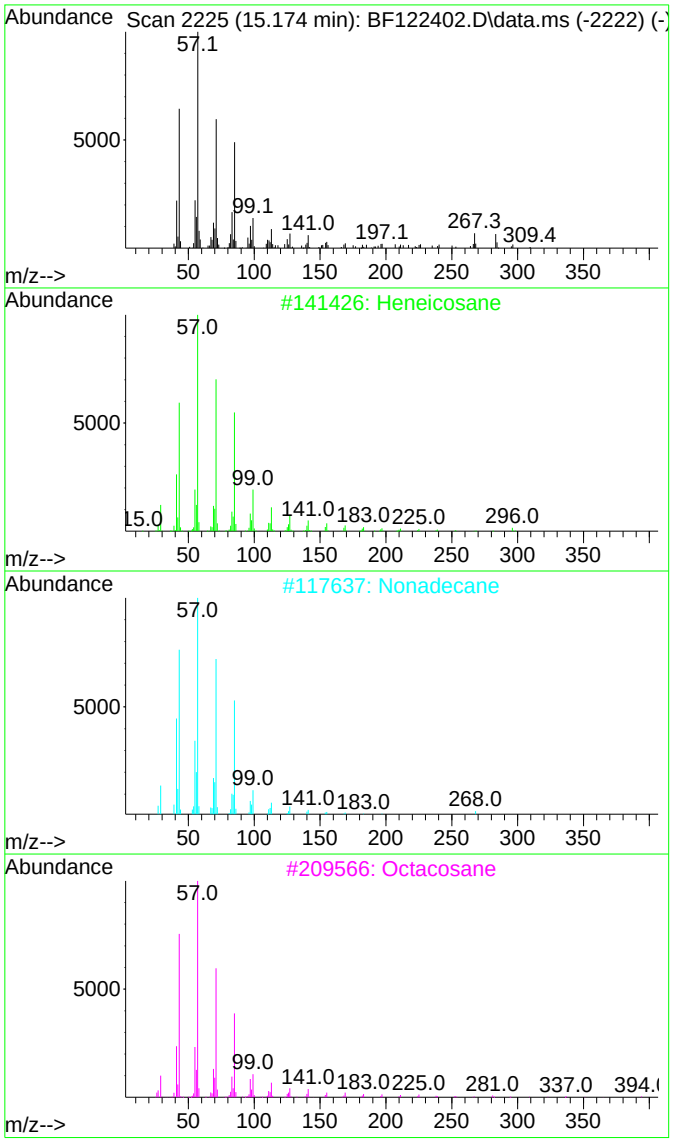
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

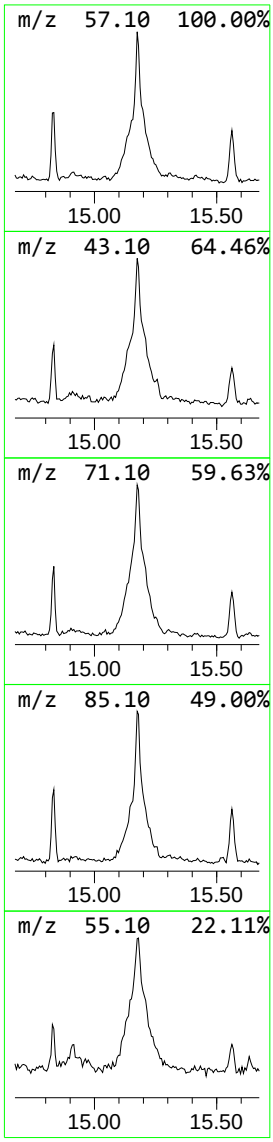
****

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	6.85 ng	801795	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Nonadecane	268	C19H40	000629-92-5	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122402.D
Acq On : 20 Nov 2020 14:34
Operator : JU/CG
Sample : L4809-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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...	2.122	11.7	ng	701241	1	6.863	1199870	20.0
4-Penten-2-one,...	3.575	37.7	ng	2264320	1	6.863	1199870	20.0
3-Penten-2-one,...	4.557	1031.3	ng	61869400	1	6.863	1199870	20.0
2-Pentanone, 4-...	5.104	143.3	ng	8600150	1	6.863	1199870	20.0
2-Cyclohexen-1-...	7.181	27.9	ng	1670520	1	6.863	1199870	20.0
Phorone	7.551	9.5	ng	738165	2	8.151	1553010	20.0
Octadecanoic acid	12.716	10.6	ng	1068280	4	11.398	2019880	20.0
Cyclopentadecane	13.898	10.2	ng	1150670	5	14.039	2266750	20.0
Heneicosane	15.174	6.8	ng	801795	6	15.521	2339790	20.0