LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-F

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: BF122407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.557	243	250	258	rBV	225243	353698	2.44%	0.731%
2	4.475	393	406	409	rBV	7487893	14509967	100.00%	29.987%
3	5.092	501	511	513	rBV	3731850	6519754	44.93%	13.474%
4	6.486	745	748	761	rBV	542289	535030	3.69%	1.106%
5	6.863	808	812	815	rBV	1590810	1235808	8.52%	2.554%
6	7.180	862	866	869	rBV	244856	194873	1.34%	0.403%
7	7.422	903	907	910	rBV	2362741	2138954	14.74%	4.420%
8	8.151	1027	1031	1034	rBV	1904194	1624457	11.20%	3.357%
9	9.227	1210	1214	1217	rBV	5064248	4256173	29.33%	8.796%
10	9.622	1277	1281	1285	rBV	182455	175654	1.21%	0.363%
11	9.910	1324	1330	1333	rBV	2384865	2067362	14.25%	4.272%
12	10.321	1396	1400	1402	rBV2	154940	167109	1.15%	0.345%
13	10.833	1482	1487	1490	rBV	576501	687080	4.74%	1.420%
14	11.298	1564	1566	1570	rVB	623314	637287	4.39%	1.317%
15	11.398	1580	1583	1589	rBV	2316384	2101076	14.48%	4.342%
16	12.992	1850	1854	1857	rBV	5019662	4666543	32.16%	9.644%
17	13.898	2006	2008	2023	rVB2	436298	906623	6.25%	1.874%
18	14.045	2029	2033	2040	rVB	2614289	2352893	16.22%	4.863%
19	15.174	2222	2225	2232	rVB	190578	237251	1.64%	0.490%
20	15.521	2279	2284	2289	rBV	1810530	2350275	16.20%	4.857%
21	16.509	2447	2452	2467	rVB2	239624	492637	3.40%	1.018%
22	17.039	2538	2542	2550	rVB2	88762	177820	1.23%	0.367%

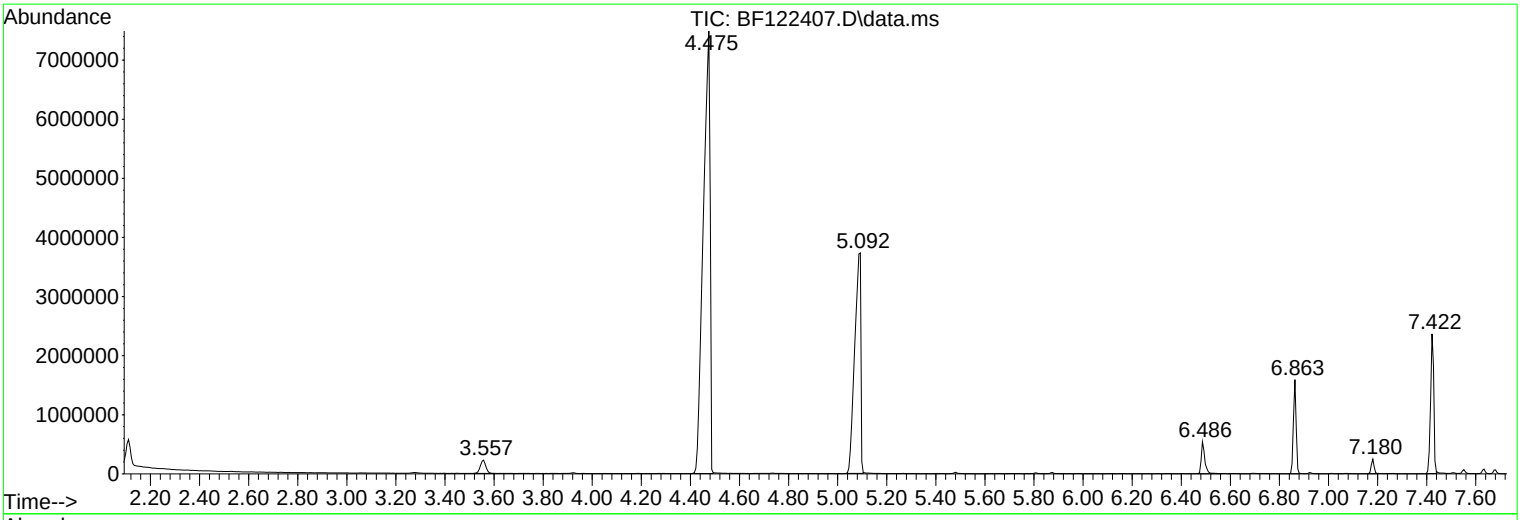
Sum of corrected areas: 48388324

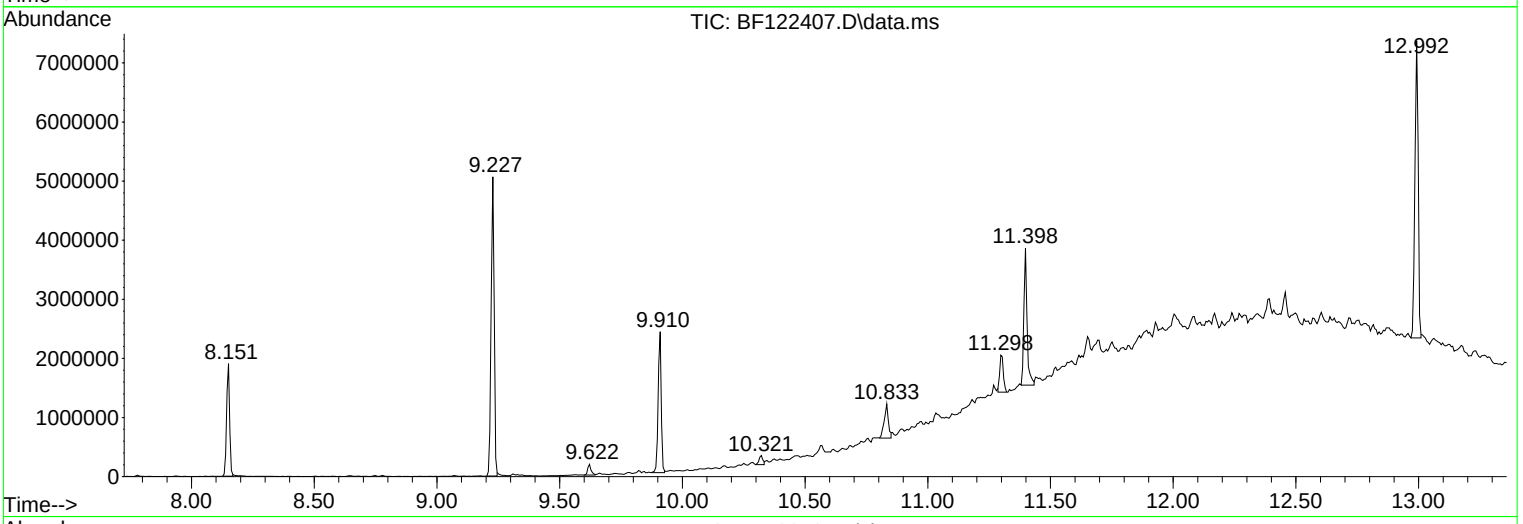
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

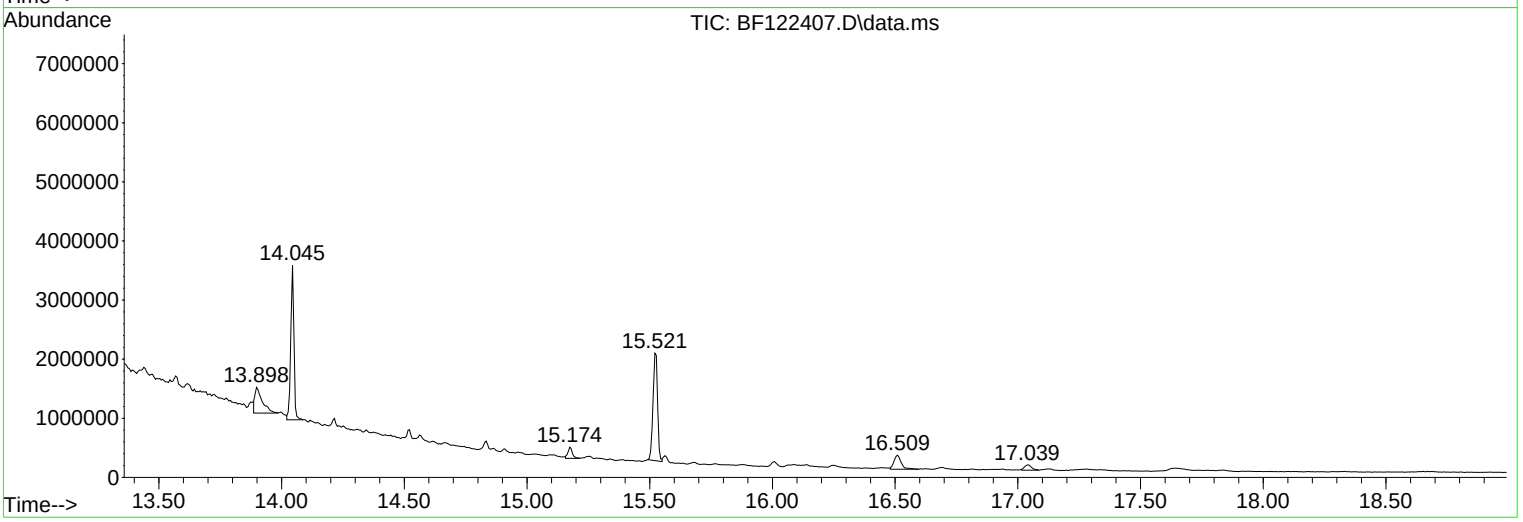
Instrument :
BNA_F
ClientSampleId :
MS-CON-F

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 : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-F

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

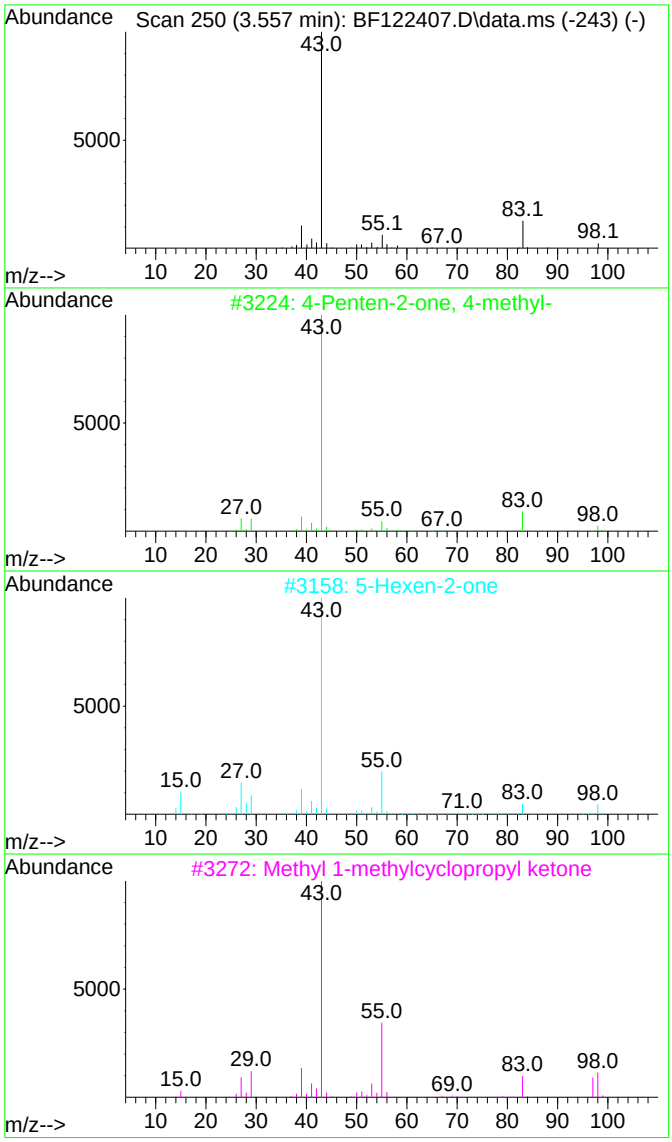
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

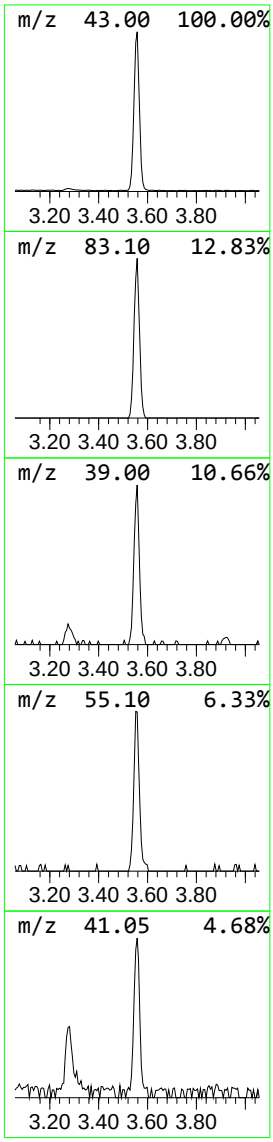
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.557	5.72 ng	353698	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	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	43
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	33
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	23
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-F

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

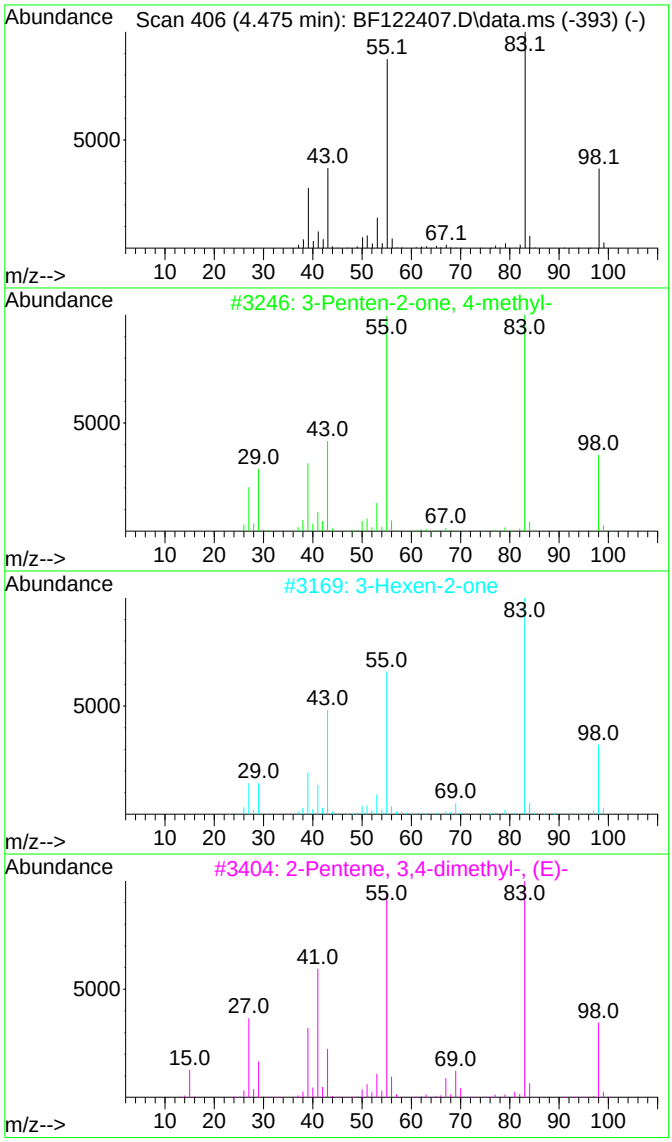
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

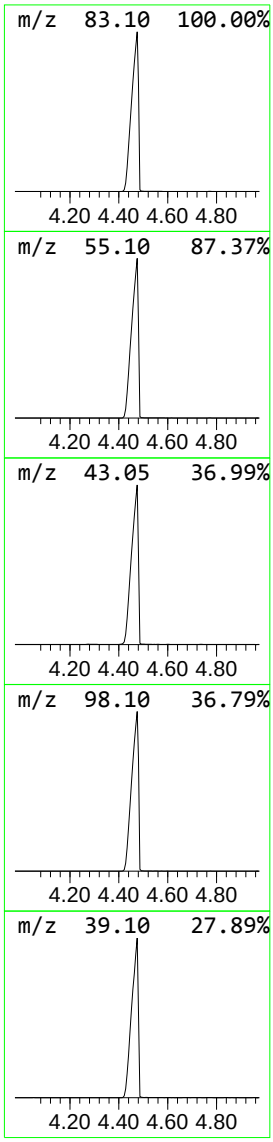
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	234.83 ng	14510000	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	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

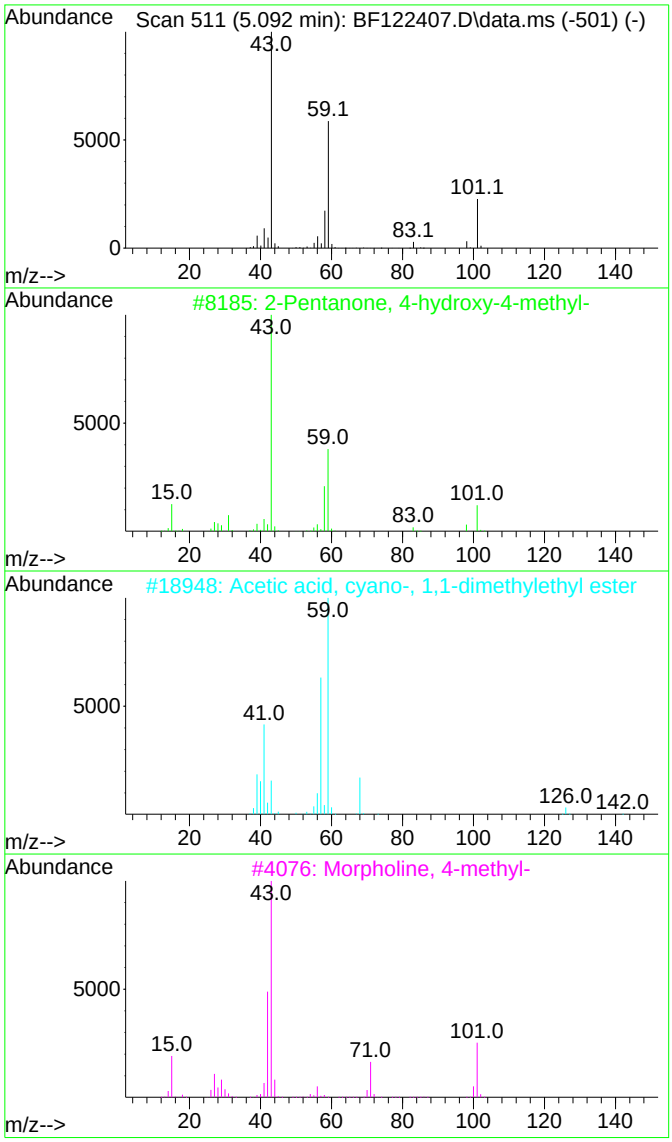
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

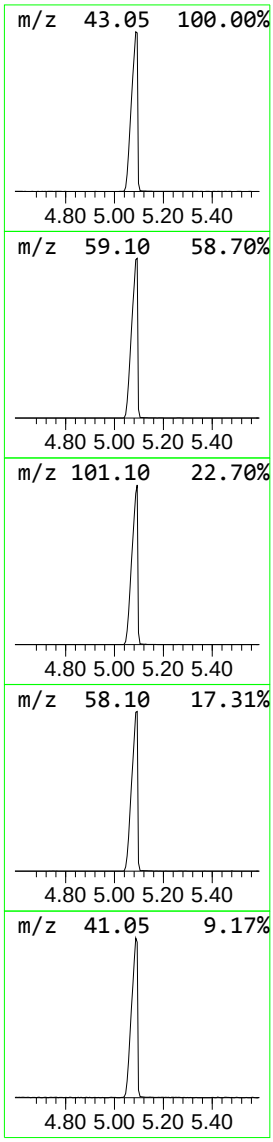
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	105.51 ng	6519750	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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

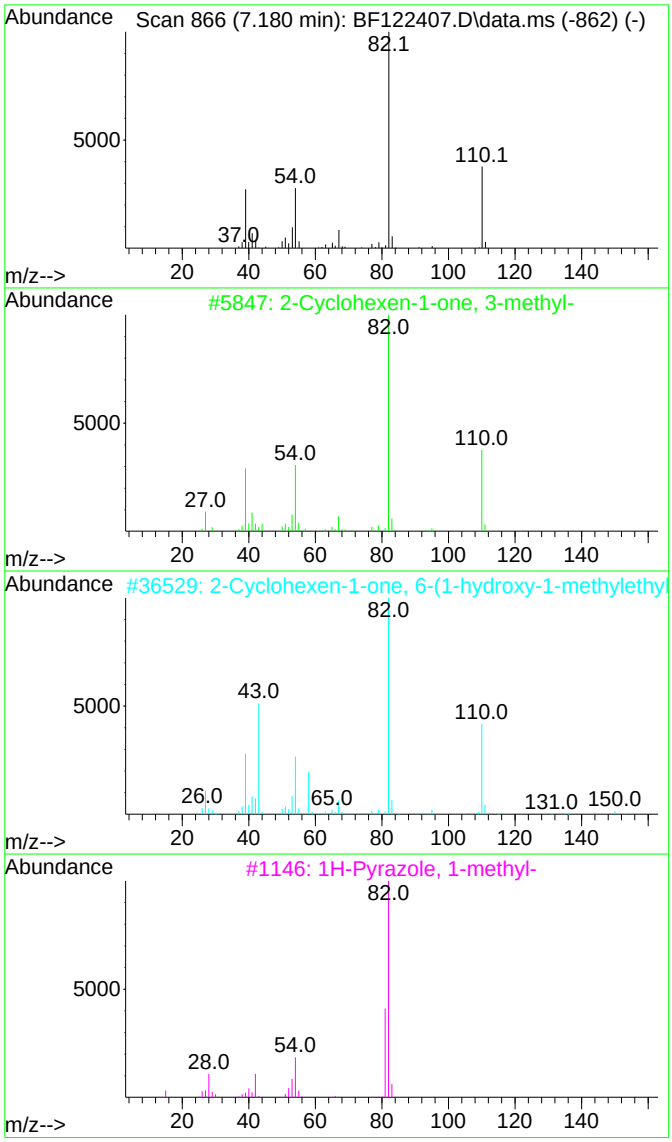
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

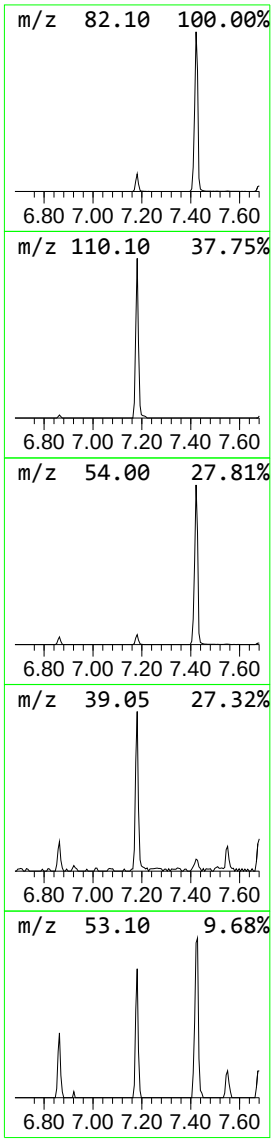
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.180	3.15 ng	194873	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, 1-methyl-	82	C4H6N2	000930-36-9	59
4	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	59
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-F

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

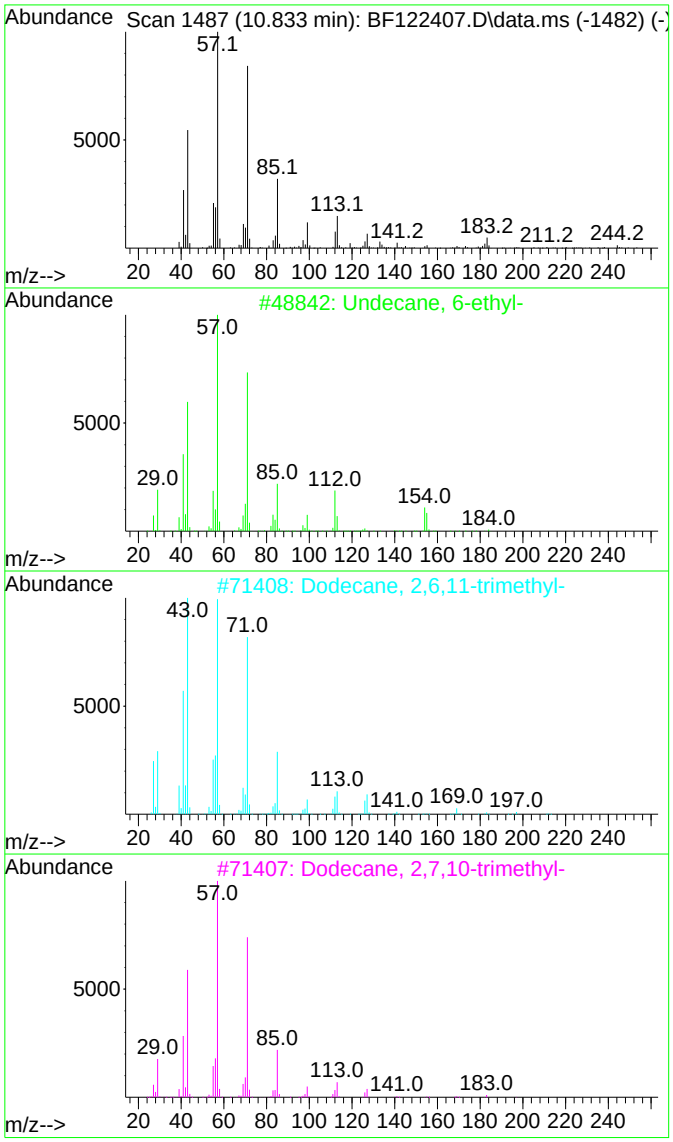
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

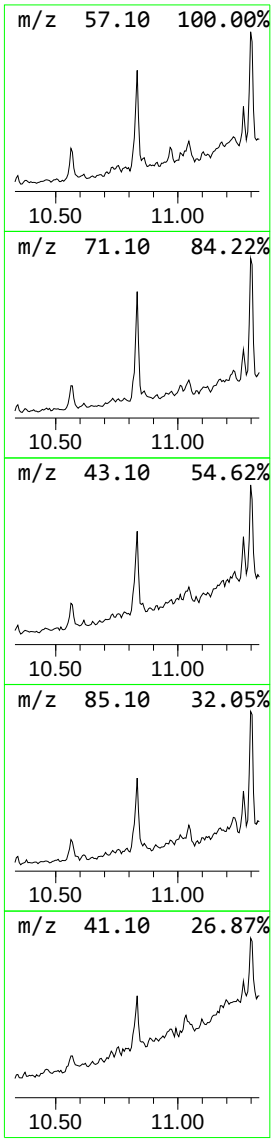
****

Peak Number 5 Undecane, 6-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	6.54 ng	687080	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-	184	C13H28	017312-60-6	90
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	74
5	Dodecane	170	C12H26	000112-40-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

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

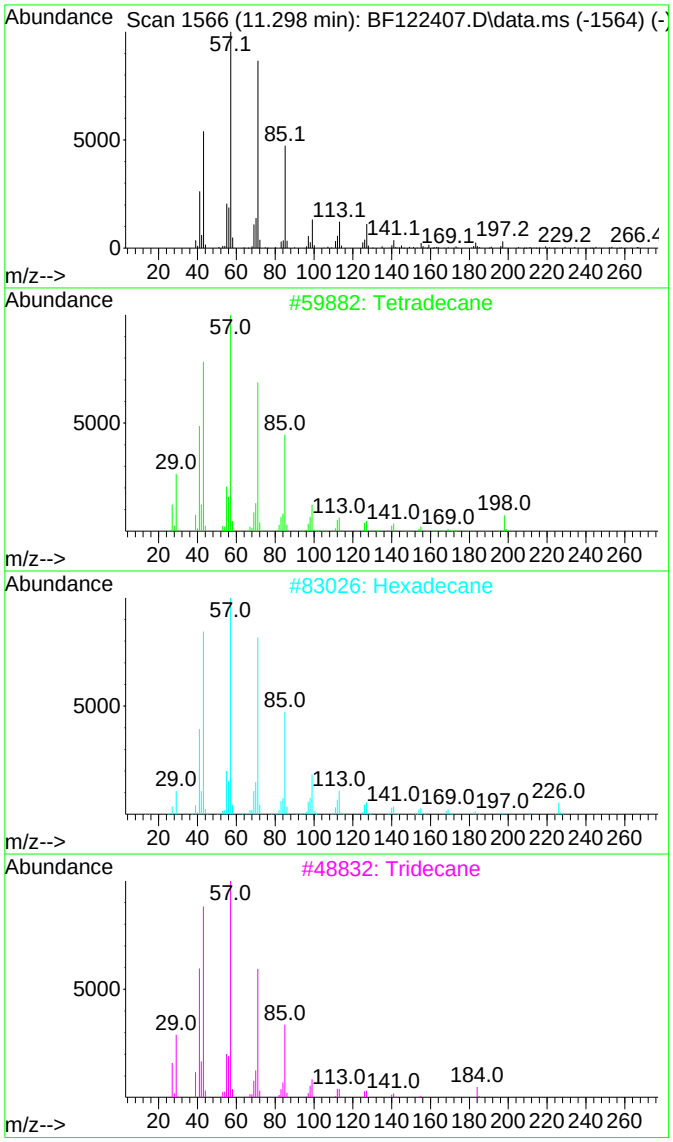
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

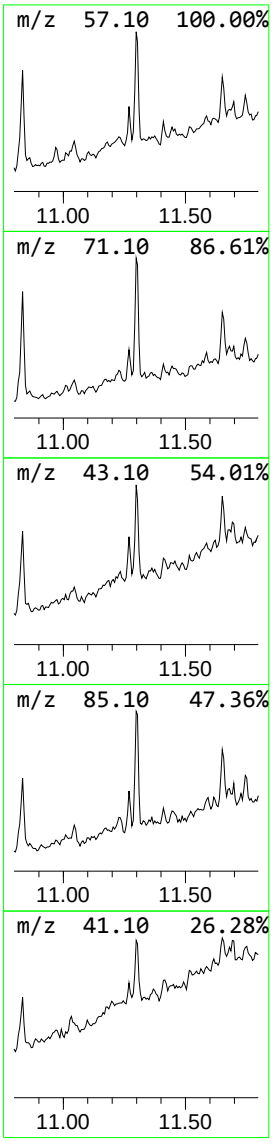
****

Peak Number 6 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	6.07 ng	637287	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	87
4	Dodecane, 4-methyl-	184	C13H28	006117-97-1	72
5	Heptacosane	380	C27H56	000593-49-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

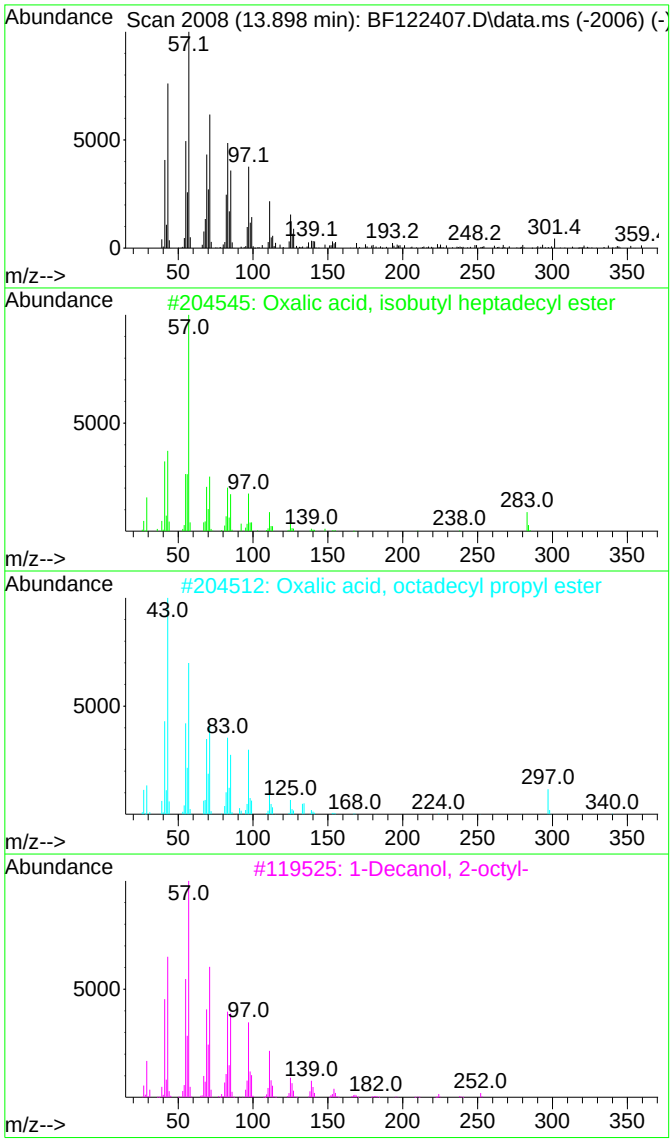
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

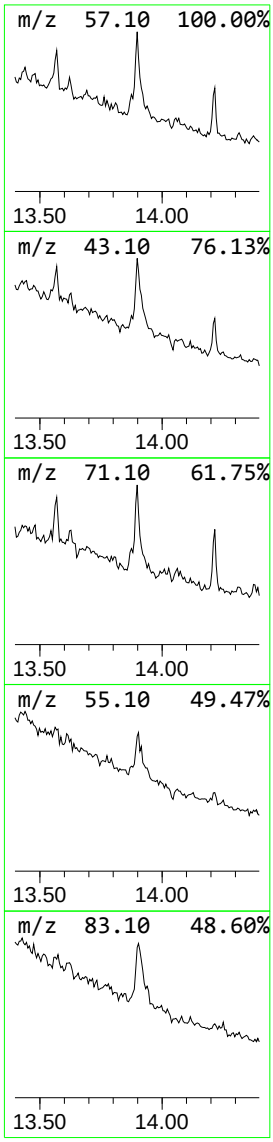
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Oxalic acid, isobutyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.71 ng	906623	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
2	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	87
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	87
4	Trihexadecyl borate	735	C48H99BO3	002665-11-4	83
5	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

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

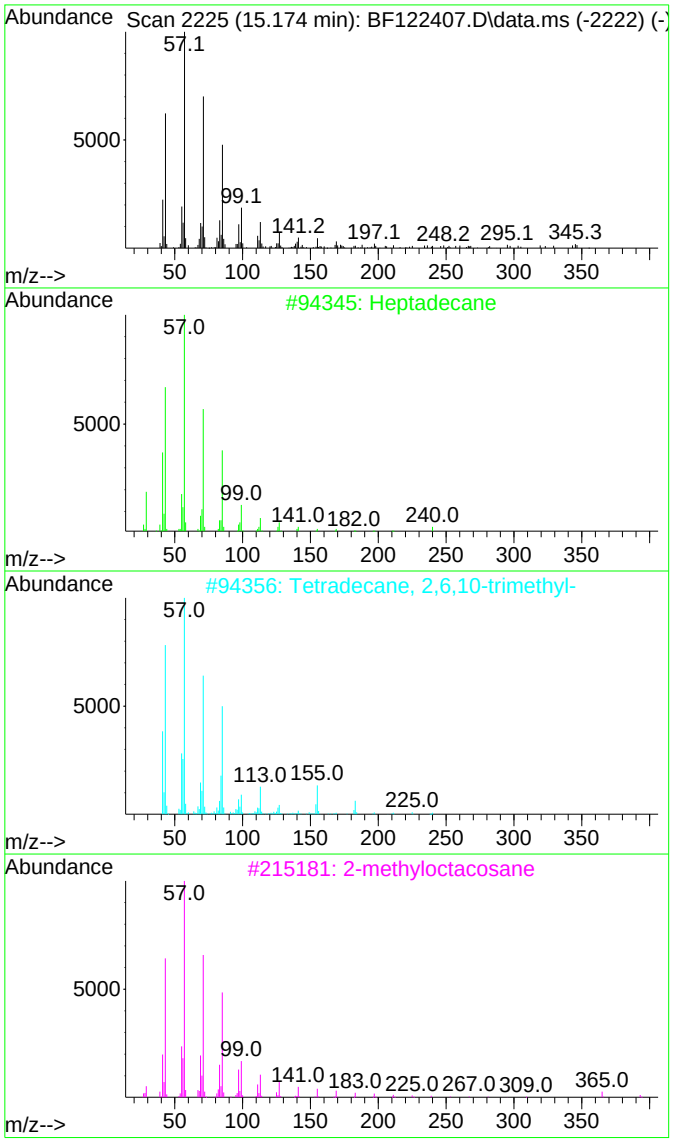
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

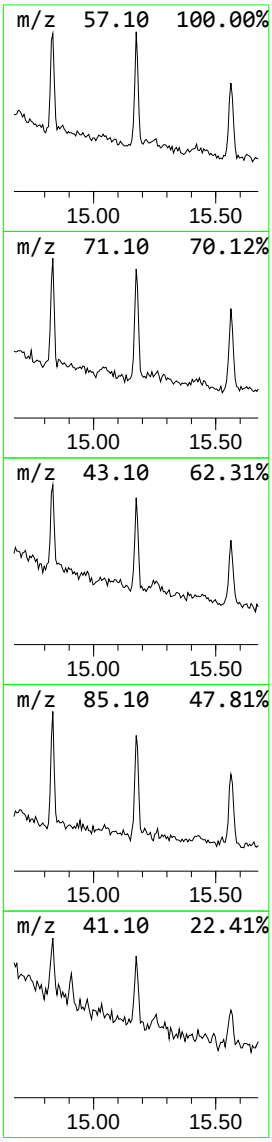
****

Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.02 ng	237251	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-CON-F

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

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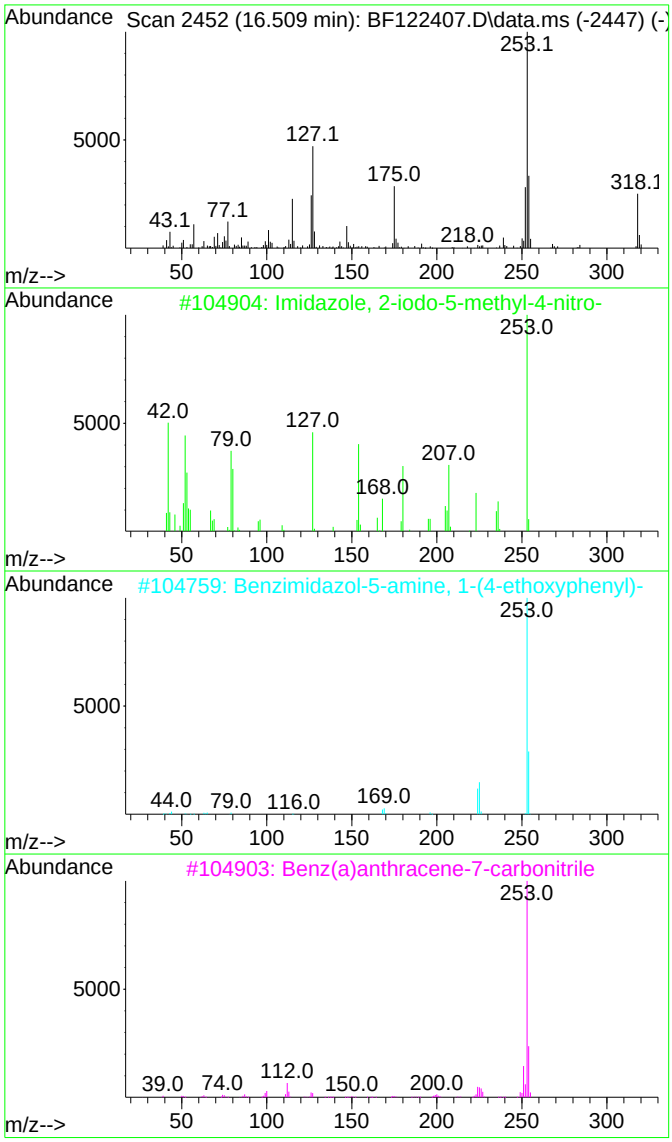
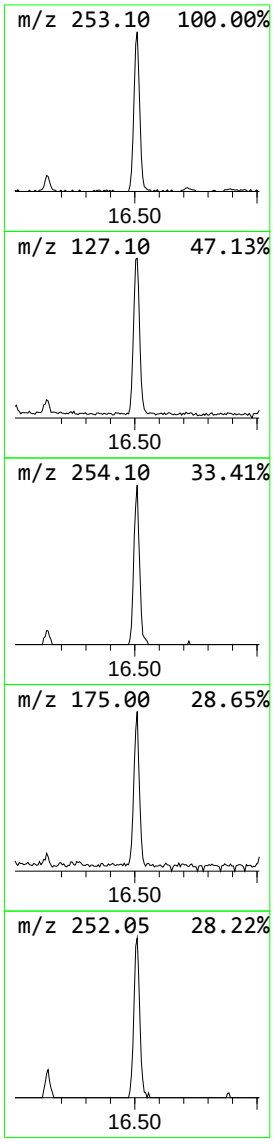
Peak Number 9 unknown16.50 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.509	4.19 ng	492637	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 2-iodo-5-methyl-4-nitro-	253	C4H4IN3O2	149510-86-1	38
2	Benzimidazol-5-amine, 1-(4-ethox...	253	C15H15N3O	007104-62-3	27
3	Benz(a)anthracene-7-carbonitrile	253	C19H11N	007476-08-6	25
4	Phthalic acid, di(2,3-dimethylph...	374	C24H22O4	1000357-09-2	10
5	7,12-Dihydrobenzo[k]fluoranthene	254	C20H14	1000080-17-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122407.D
Acq On : 20 Nov 2020 17:11
Operator : JU/CG
Sample : L4809-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MS-CON-F

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
4-Penten-2-one,...	3.557	5.7	ng	353698	1	6.863	1235810	20.0
3-Penten-2-one,...	4.475	234.8	ng	14510000	1	6.863	1235810	20.0
2-Pentanone, 4-...	5.092	105.5	ng	6519750	1	6.863	1235810	20.0
2-Cyclohexen-1-...	7.180	3.1	ng	194873	1	6.863	1235810	20.0
Undecane, 6-ethyl-	10.833	6.5	ng	687080	4	11.398	2101080	20.0
Tetradecane	11.298	6.1	ng	637287	4	11.398	2101080	20.0
Oxalic acid, is...	13.898	7.7	ng	906623	5	14.045	2352890	20.0
Heptadecane	15.174	2.0	ng	237251	6	15.527	2350280	20.0
unknown16.50	16.509	4.2	ng	492637	6	15.527	2350280	20.0