LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129698.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.151	313	317	327	rBV	70742	103325	1.15%	0.169%
2	4.363	348	353	363	rBV	1400256	1785747	19.87%	2.917%
3	4.457	363	369	377	rVV	2618294	2978191	33.14%	4.865%
4	5.075	469	474	491	rVB	1104739	1391677	15.49%	2.273%
5	5.487	540	544	559	rVB	4213159	4061220	45.19%	6.634%
6	6.140	651	655	658	rBV	569843	506828	5.64%	0.828%
7	6.493	711	715	722	rVB	2951057	2758734	30.70%	4.506%
8	6.834	769	773	777	rBV	2090076	1793332	19.96%	2.929%
9	6.898	781	784	790	rBV	840757	824209	9.17%	1.346%
10	6.987	796	799	809	rVB	91818	122941	1.37%	0.201%
11	7.240	832	842	852	rVB2	209333	401296	4.47%	0.656%
12	7.410	861	871	874	rBV	4203811	5030173	55.97%	8.217%
13	7.516	885	889	894	rVB2	69981	97438	1.08%	0.159%
14	7.651	908	912	916	rBV	338927	311129	3.46%	0.508%
15	7.898	944	954	962	rBV3	326409	666532	7.42%	1.089%
16	8.028	972	976	983	rBV2	97376	139586	1.55%	0.228%
17	8.122	987	992	995	rBV	2499976	2440949	27.16%	3.987%
18	8.434	1041	1045	1050	rBV	109065	140724	1.57%	0.230%
19	8.504	1050	1057	1060	rVV2	568839	745099	8.29%	1.217%
20	8.563	1063	1067	1071	rVV	181952	218118	2.43%	0.356%
21	9.075	1151	1154	1157	rBV2	66275	95439	1.06%	0.156%
22	9.116	1157	1161	1166	rVB2	78194	105196	1.17%	0.172%
23	9.198	1166	1175	1178	rBV	8522367	8986554	100.00%	14.680%
24	9.304	1188	1193	1200	rVB	3383471	2949469	32.82%	4.818%
25	9.875	1282	1290	1294	rBV	2968281	2801852	31.18%	4.577%
26	10.286	1358	1360	1364	rVB	130238	121376	1.35%	0.198%
27	10.451	1384	1388	1392	rVB	111951	107816	1.20%	0.176%
28	10.580	1406	1410	1412	rBV	177942	158315	1.76%	0.259%
29	10.675	1417	1426	1429	rBV	5225271	5672567	63.12%	9.266%
30	11.369	1536	1544	1547	rBV	2951573	2560735	28.50%	4.183%
31	11.739	1604	1607	1610	rVB	273317	221933	2.47%	0.363%
32	12.957	1809	1814	1817	rBV	7308437	7595226	84.52%	12.407%
33	14.016	1990	1994	1997	rBV	1530864	1443578	16.06%	2.358%
34	14.098	2003	2008	2014	rBV	344094	394794	4.39%	0.645%
35	15.492	2239	2245	2250	rVB	1156045	1486232	16.54%	2.428%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

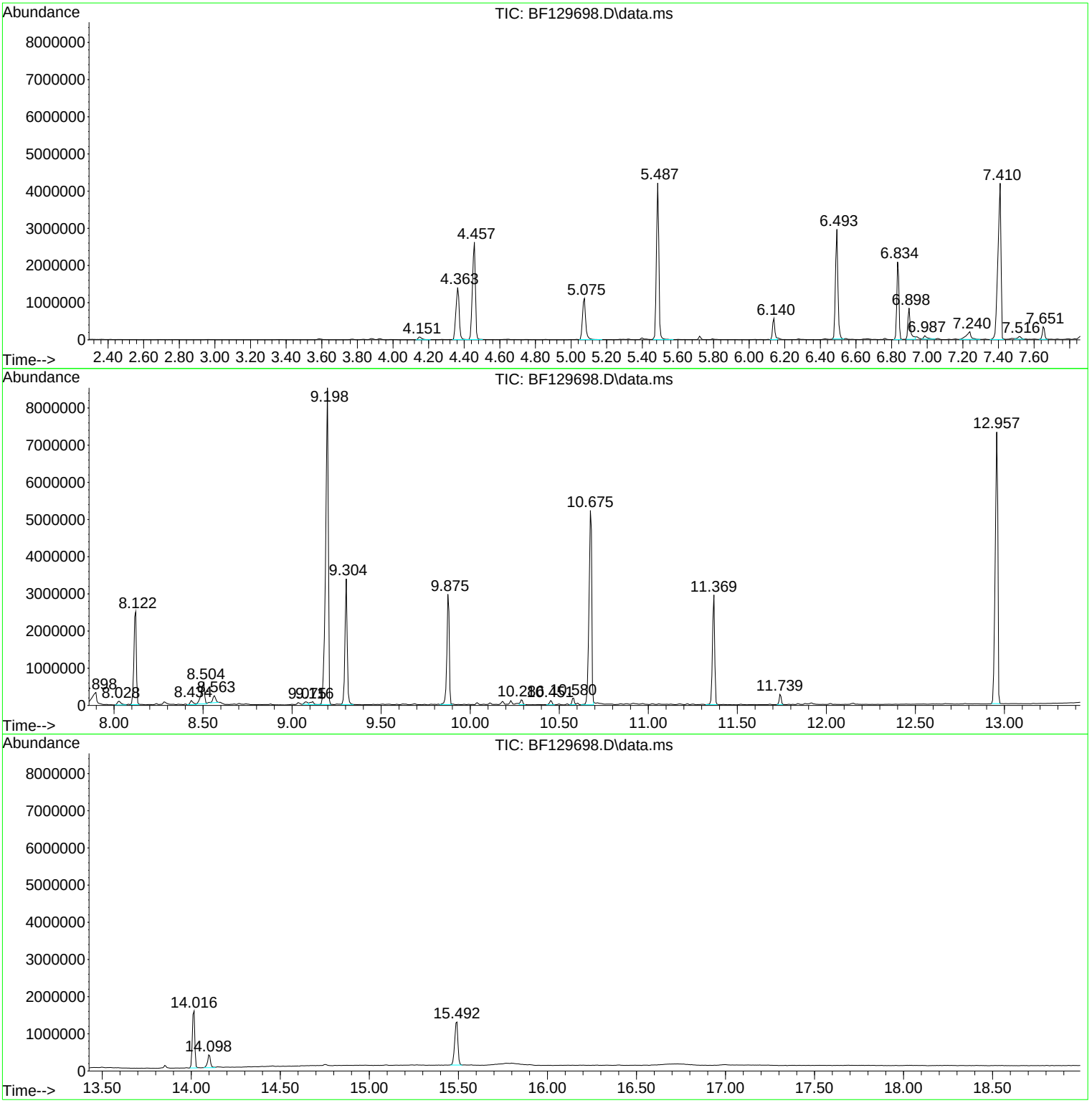
Sum of corrected areas: 61218330

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

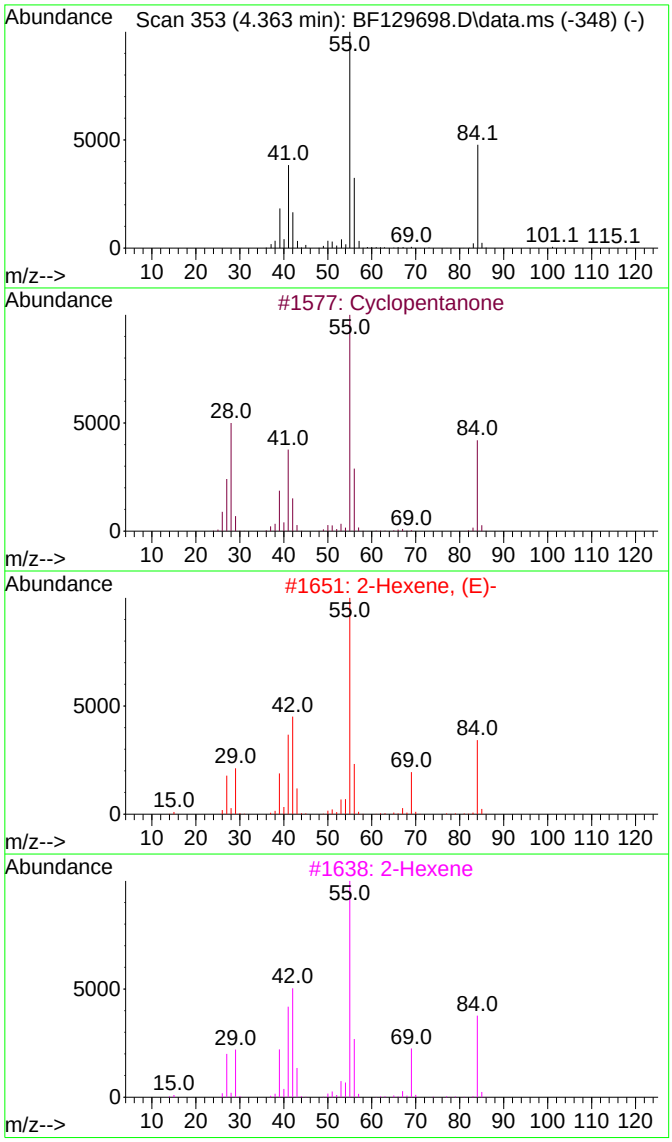
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

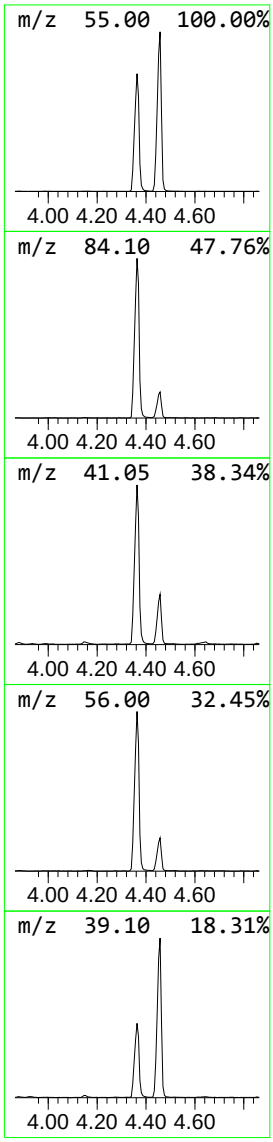
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.363	19.92 ng	1785750	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	90
2	2-Hexene, (E)-	84	C6H12	004050-45-7	64
3	2-Hexene	84	C6H12	000592-43-8	64
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	49
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

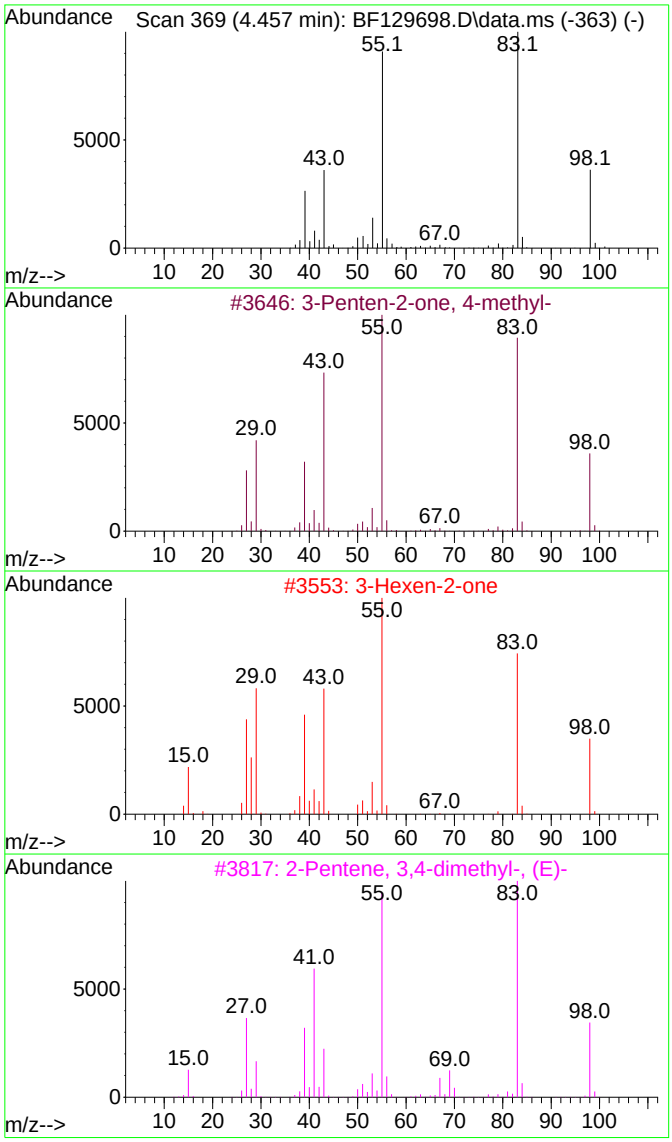
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

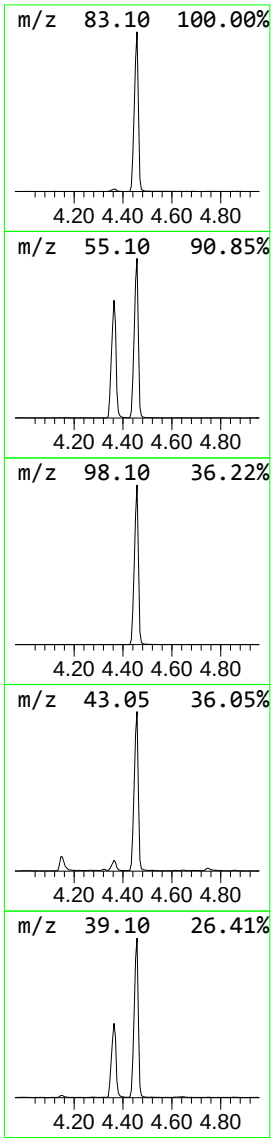
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	33.21 ng	2978190	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
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\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

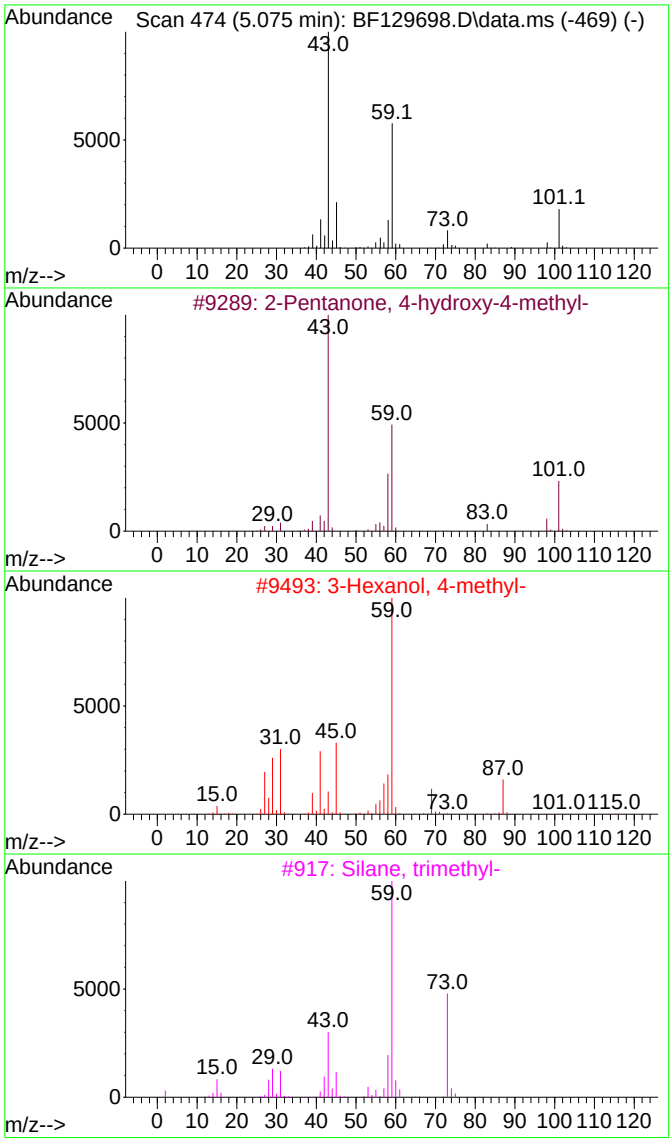
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

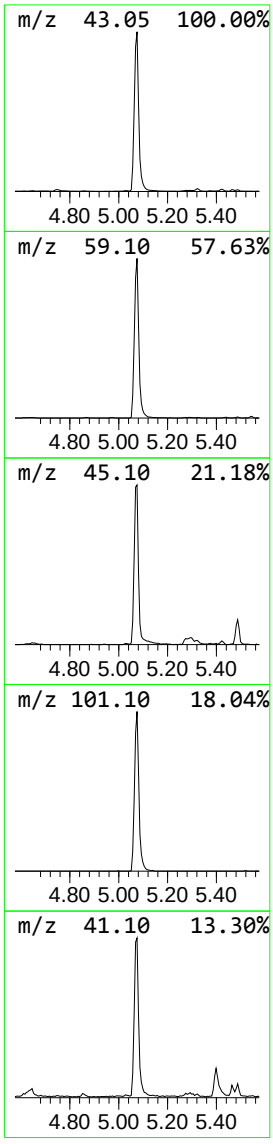
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	15.52 ng	1391680	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	38
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	38
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	37
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

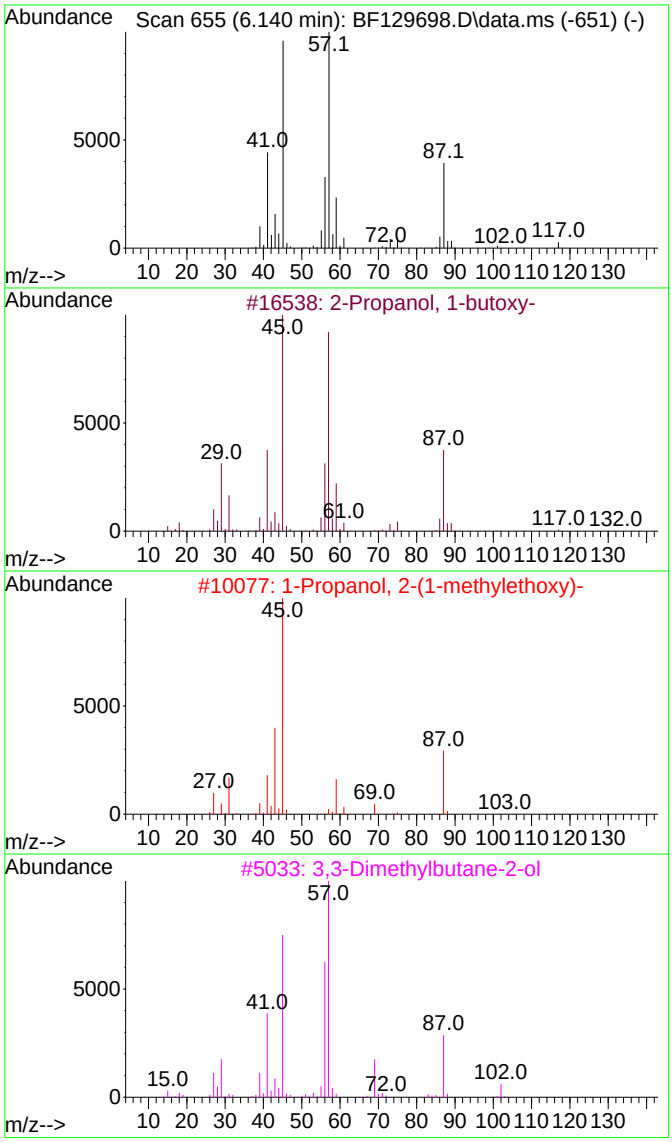
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

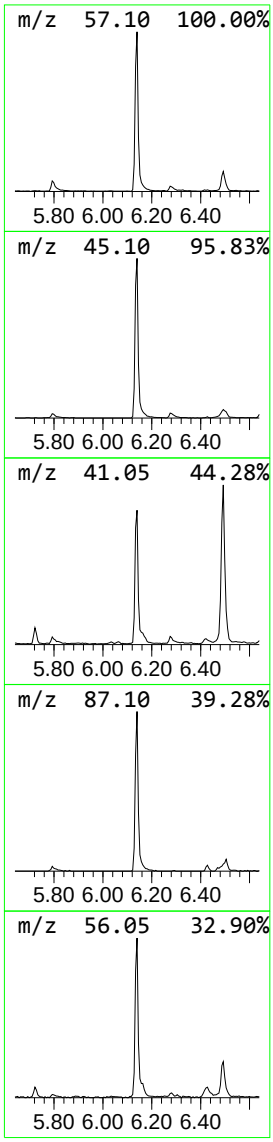
****

Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.140	5.65 ng	506828	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	50
5	Diisopropyl ether	102	C6H14O	000108-20-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
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Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

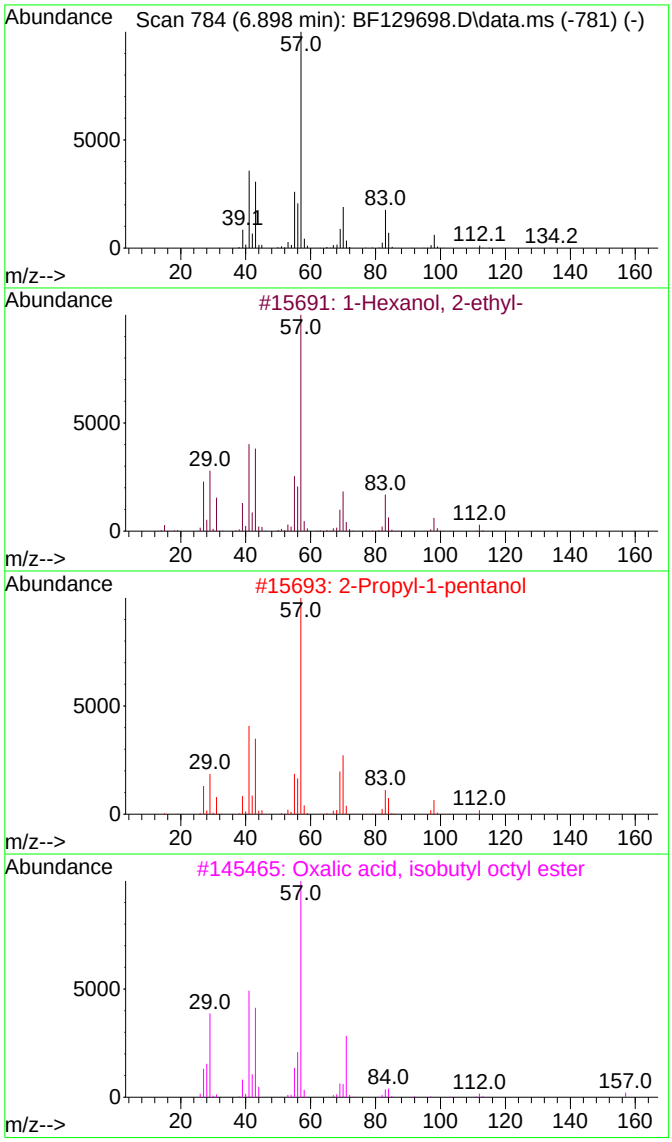
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

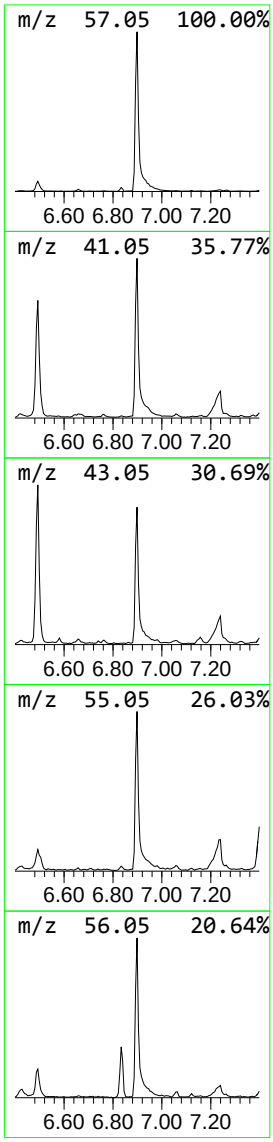
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.898	9.19 ng	824209	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50





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Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

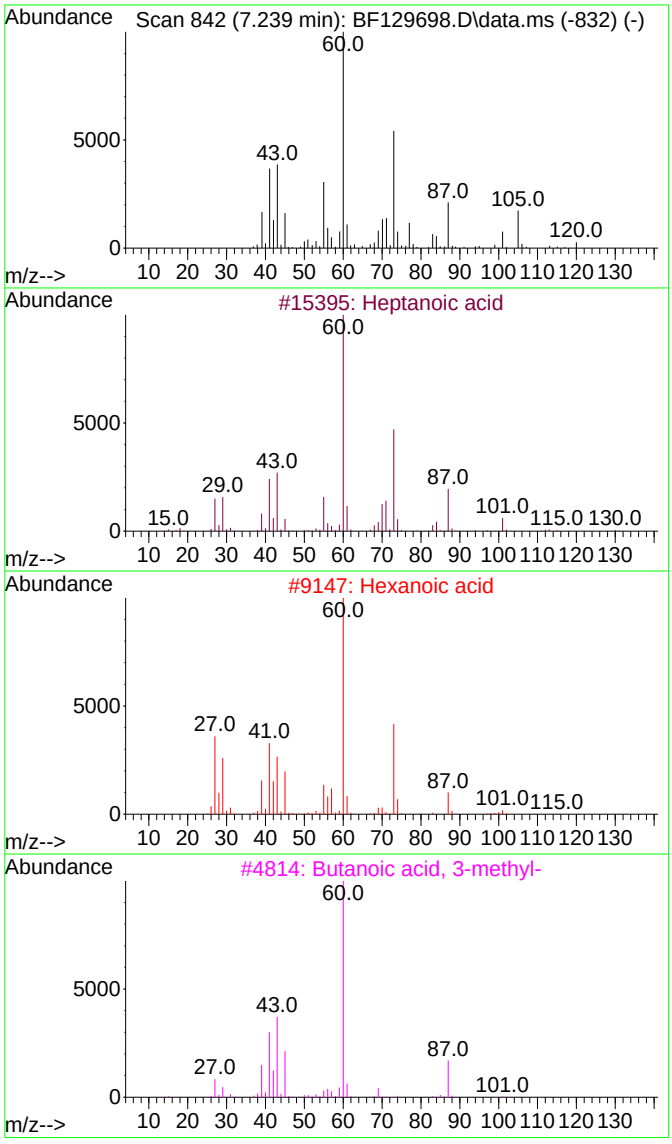
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

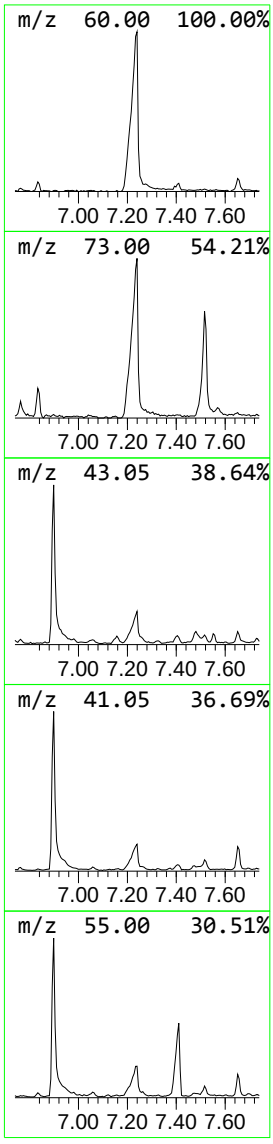
****

Peak Number 6 Heptanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.239	4.48 ng	401296	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	80
2	Hexanoic acid	116	C6H12O2	000142-62-1	53
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	43
5	Octanoic acid	144	C8H16O2	000124-07-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

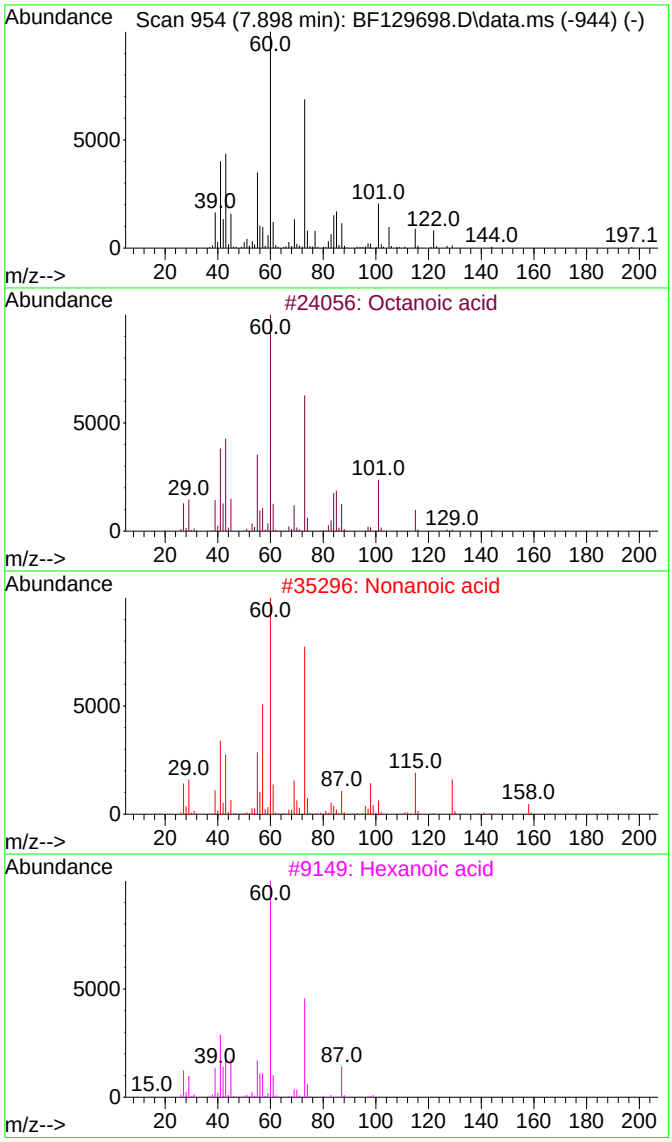
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

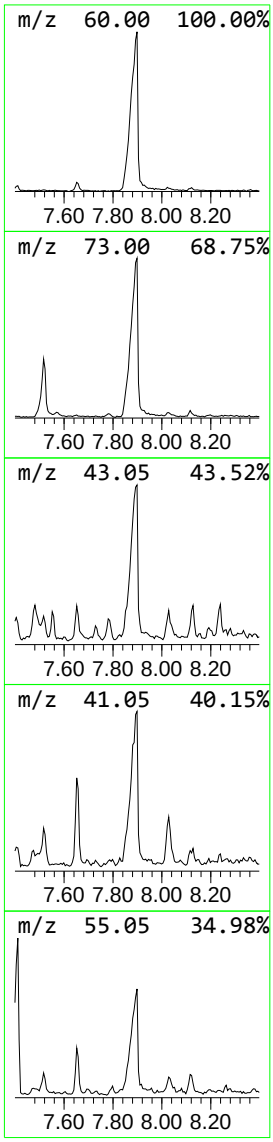
****

Peak Number 7 Octanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	5.46 ng	666532	Naphthalene-d8	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	97
2	Nonanoic acid	158	C9H18O2	000112-05-0	53
3	Hexanoic acid	116	C6H12O2	000142-62-1	53
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47





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Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

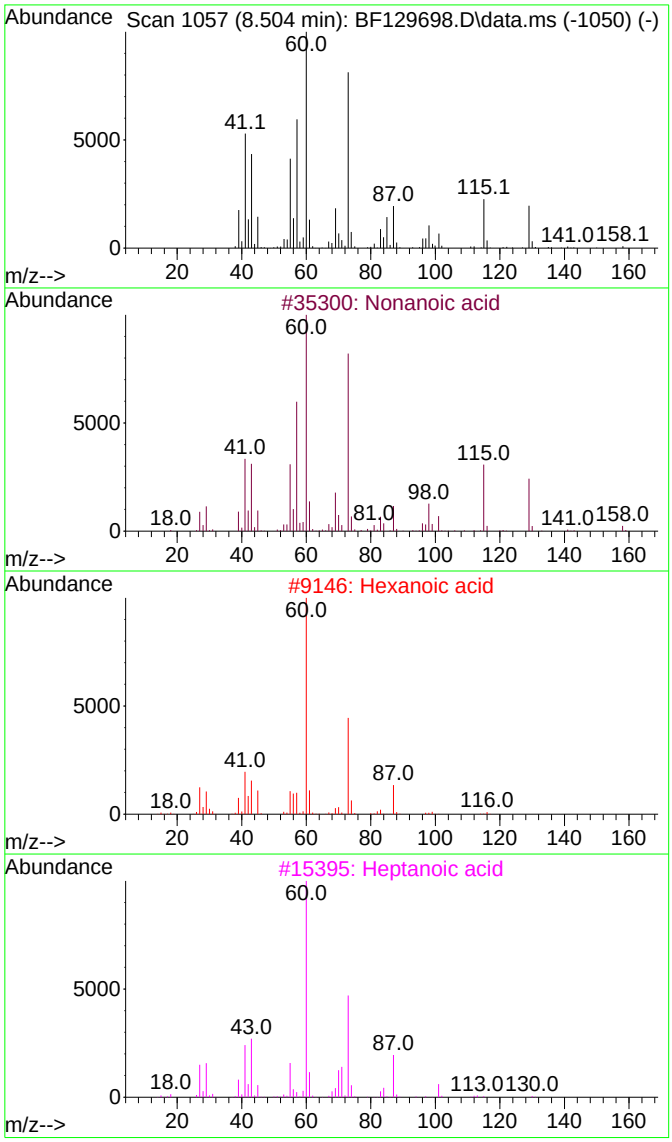
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

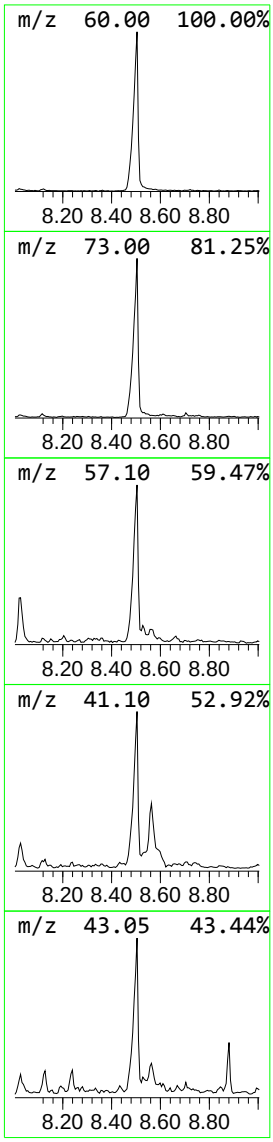
****

Peak Number 8 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.504	6.10 ng	745099	Naphthalene-d8	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	93
2	Hexanoic acid	116	C6H12O2	000142-62-1	47
3	Heptanoic acid	130	C7H14O2	000111-14-8	47
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
5	Octanoic acid	144	C8H16O2	000124-07-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

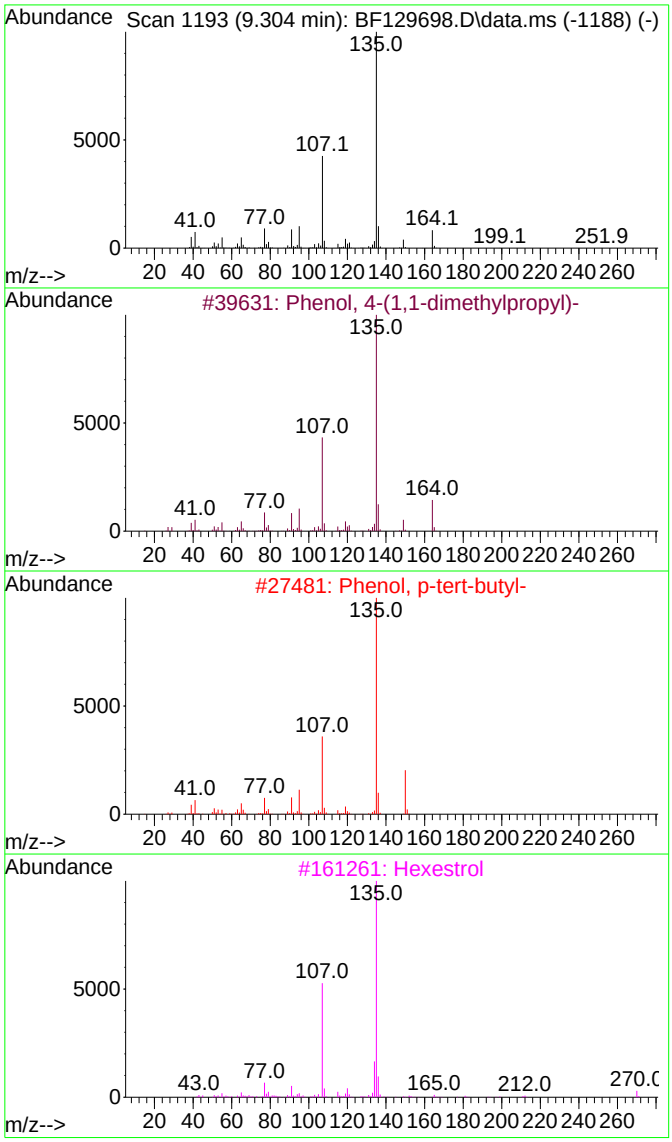
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

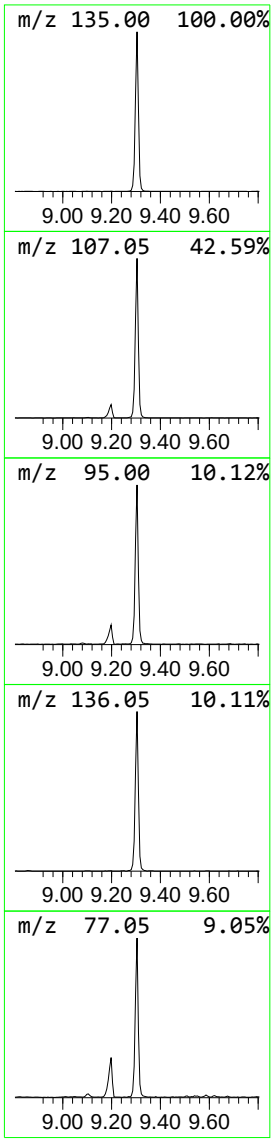
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	21.05 ng	2949470	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Hexestrol	270	C18H22O2	000084-16-2	72
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
5	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

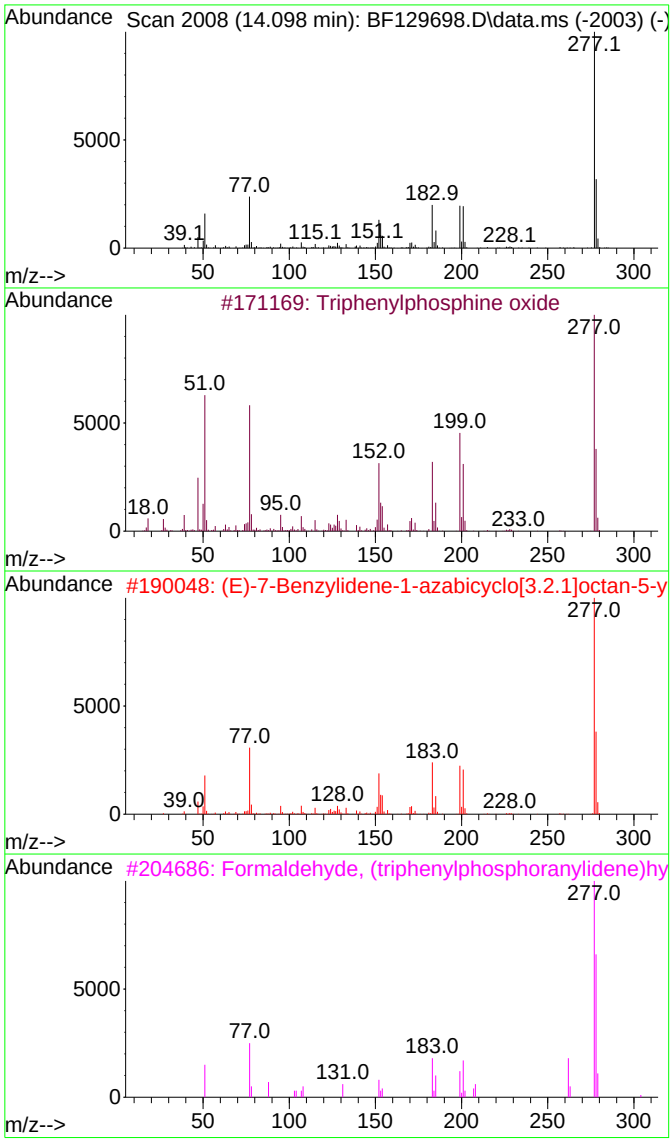
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

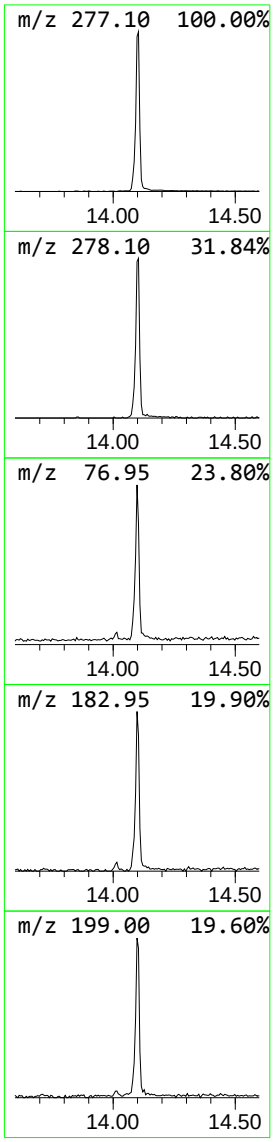
****

Peak Number 10 Triphenylphosphine oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	5.47 ng	394794	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081022\
Data File : BF129698.D
Acq On : 10 Aug 2022 16:37
Operator : CG\JU
Sample : N3971-19
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentanone	4.363	19.9	ng	1785750	1	6.834	1793330	20.0
3-Penten-2-one,...	4.457	33.2	ng	2978190	1	6.834	1793330	20.0
2-Pentanone, 4-...	5.075	15.5	ng	1391680	1	6.834	1793330	20.0
2-Propanol, 1-b...	6.140	5.7	ng	506828	1	6.834	1793330	20.0
1-Hexanol, 2-et...	6.898	9.2	ng	824209	1	6.834	1793330	20.0
Heptanoic acid	7.239	4.5	ng	401296	1	6.834	1793330	20.0
Octanoic acid	7.898	5.5	ng	666532	2	8.122	2440950	20.0
Nonanoic acid	8.504	6.1	ng	745099	2	8.122	2440950	20.0
Phenol, 4-(1,1-...	9.304	21.1	ng	2949470	3	9.875	2801850	20.0
Triphenylphosph...	14.098	5.5	ng	394794	5	14.015	1443580	20.0