LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

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-BP010820.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	2.899	14	19	28	rBV	82008	155678	5.57%	0.876%
2	2.975	28	32	47	rVB	135084	210641	7.54%	1.186%
3	4.828	342	347	356	rBV	167132	245220	8.78%	1.380%
4	5.287	419	425	435	rBV	785358	1182184	42.32%	6.655%
5	6.857	683	692	705	rBV	939091	1516495	54.28%	8.537%
6	7.204	743	751	759	rVB	892942	1388313	49.70%	7.815%
7	7.657	821	828	835	rBV	151073	237627	8.51%	1.338%
8	7.975	874	882	890	rBV	645289	1020562	36.53%	5.745%
9	8.804	1014	1023	1035	rBV	592049	961136	34.40%	5.411%
10	10.433	1292	1300	1311	rBV	204445	334399	11.97%	1.882%
11	12.922	1716	1723	1733	rVB	1341577	1899808	68.01%	10.695%
12	13.769	1862	1867	1875	rBV	45099	61320	2.19%	0.345%
13	14.304	1950	1958	1965	rBV	313788	476491	17.06%	2.682%
14	15.804	2205	2213	2225	rBV	1269031	1888238	67.59%	10.630%
15	17.063	2419	2427	2431	rBV	431544	619583	22.18%	3.488%
16	17.104	2431	2434	2440	rVB	29693	39851	1.43%	0.224%
17	17.192	2445	2449	2455	rVB2	28168	37364	1.34%	0.210%
18	17.998	2580	2586	2592	rBV2	107300	153030	5.48%	0.861%
19	18.968	2747	2751	2759	rBV	17988	31442	1.13%	0.177%
20	19.080	2766	2770	2774	rBV	124126	183015	6.55%	1.030%
21	19.127	2774	2778	2793	rVV2	147670	255813	9.16%	1.440%
22	19.245	2794	2798	2806	rVB	53454	80512	2.88%	0.453%
23	19.433	2823	2830	2834	rBV	97756	130549	4.67%	0.735%
24	19.651	2861	2867	2872	rBV	2415210	2793627	100.00%	15.726%
25	20.292	2972	2976	2982	rBV3	51866	81597	2.92%	0.459%
26	20.915	3078	3082	3094	rVB2	90459	117589	4.21%	0.662%
27	21.162	3118	3124	3128	rBV	550110	760695	27.23%	4.282%
28	21.198	3128	3130	3139	rVB	52762	67302	2.41%	0.379%
29	22.262	3309	3311	3316	rVB2	39111	43314	1.55%	0.244%
30	22.392	3330	3333	3338	rVB	52628	67354	2.41%	0.379%
31	22.733	3388	3391	3395	rBV2	34624	57749	2.07%	0.325%
32	23.415	3501	3507	3520	rVB	321439	665436	23.82%	3.746%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4F-(22-24)

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-BP010820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

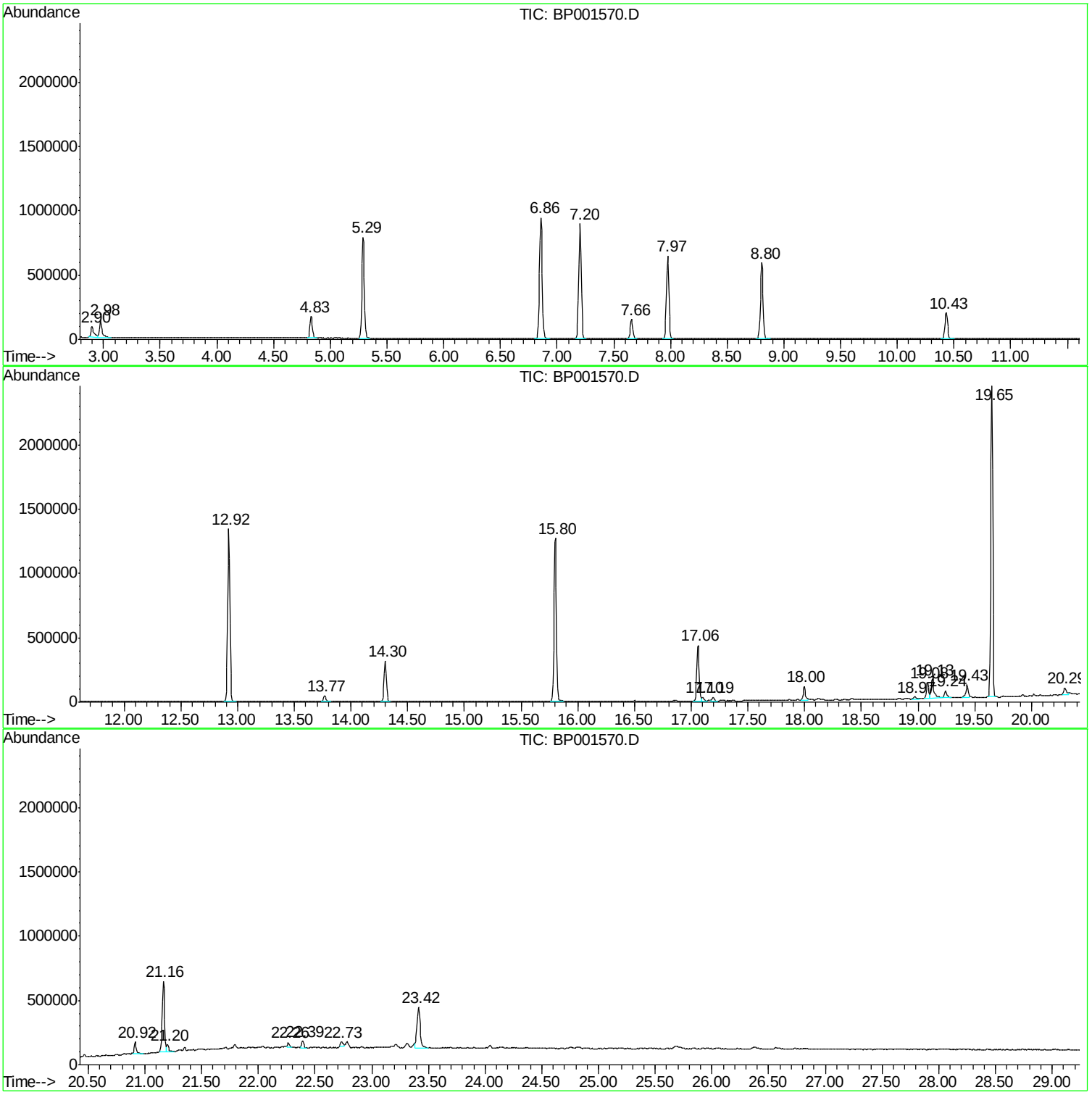
Sum of corrected areas: 17763934

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

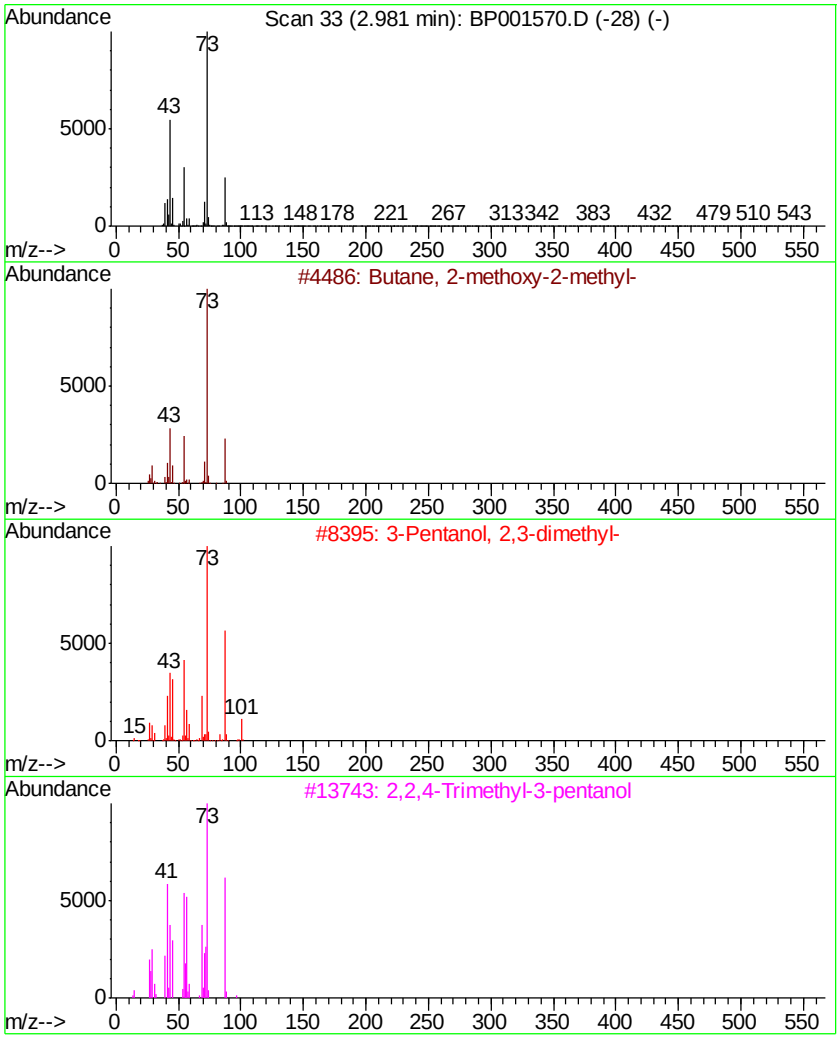
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

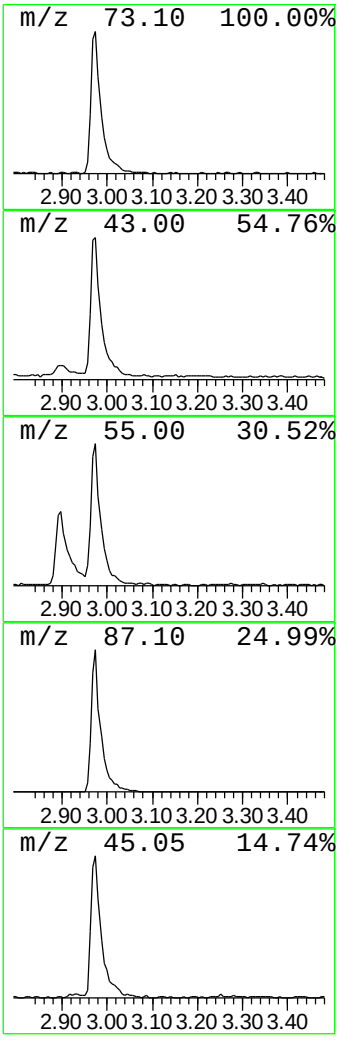
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	17.73 ng	210641	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	53
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	37
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

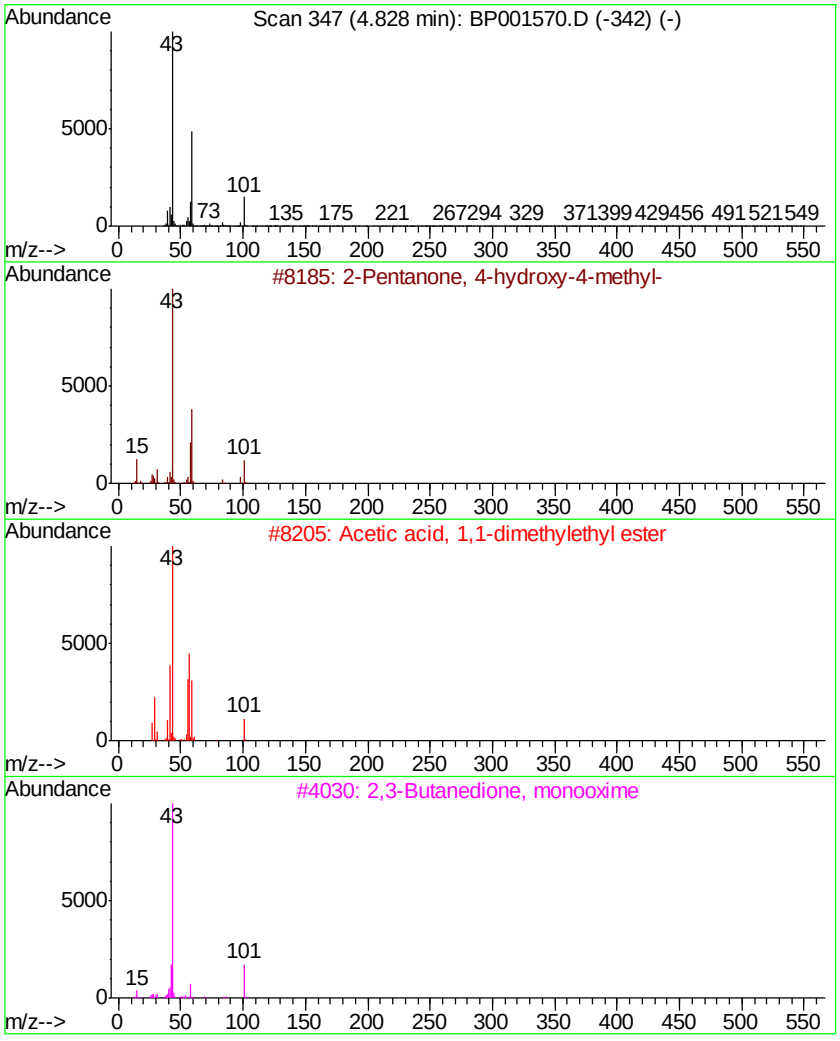
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

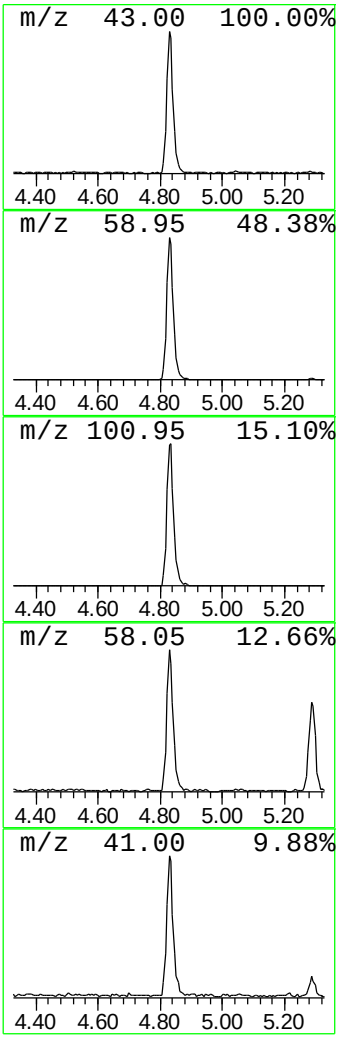
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	20.64 ng	245220	1,4-Dichlorobenzene-d4	7.66

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

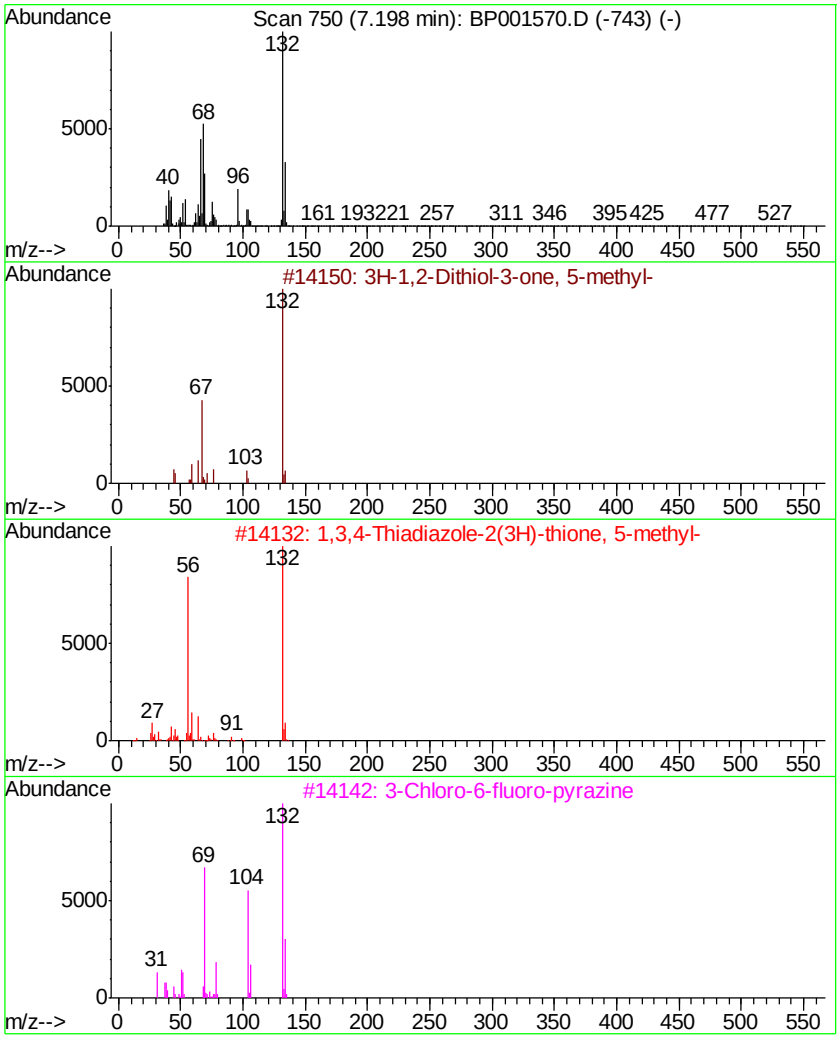
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

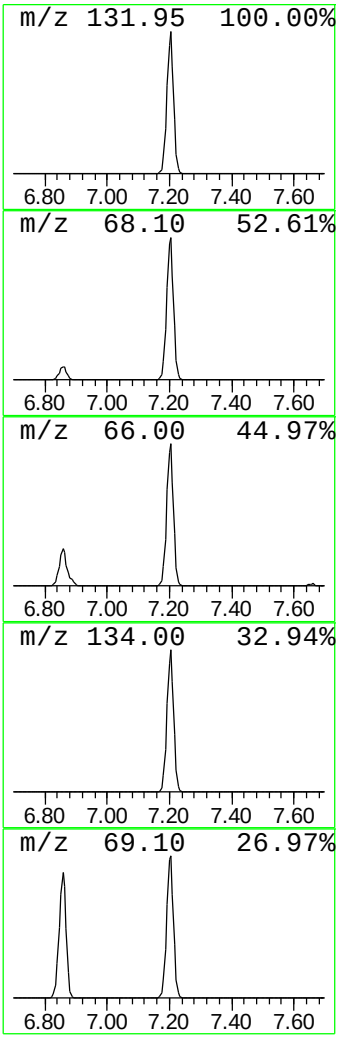
****

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	116.85 ng	1388310	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

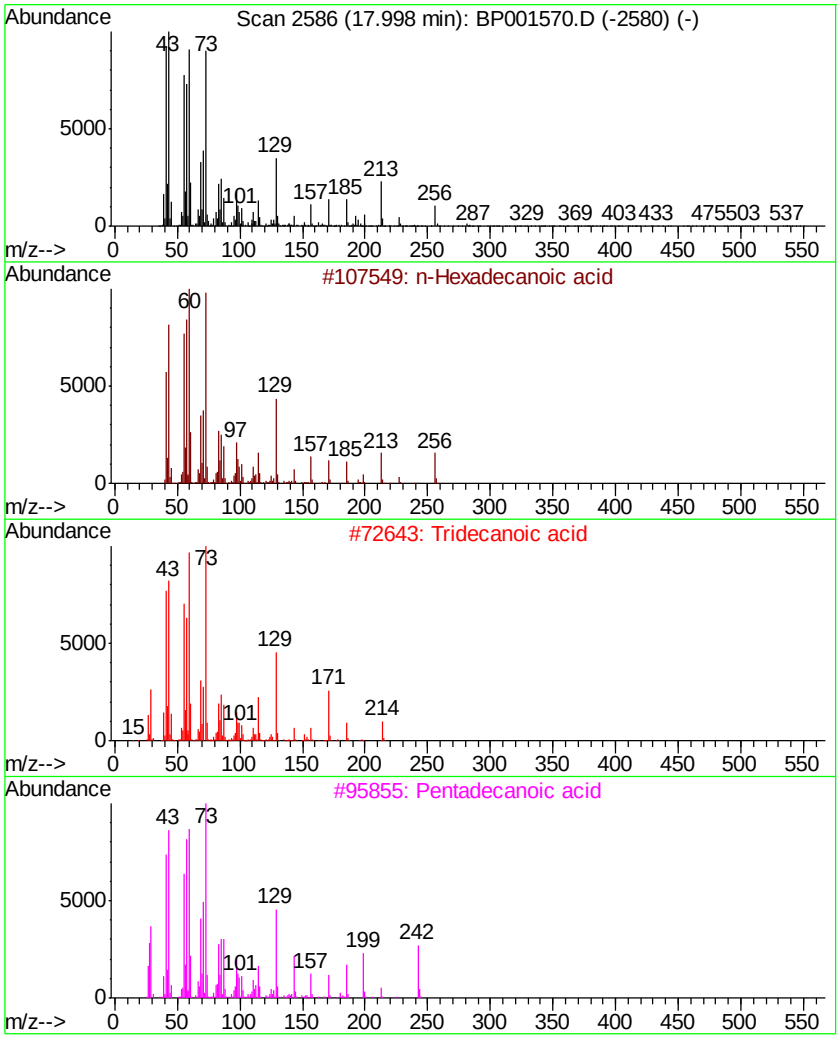
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

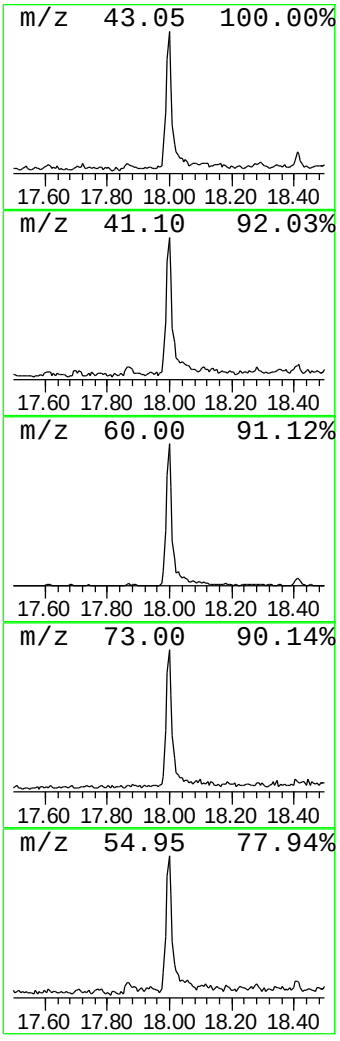
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	4.94 ng	153030	Phenanthrene-d10	17.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

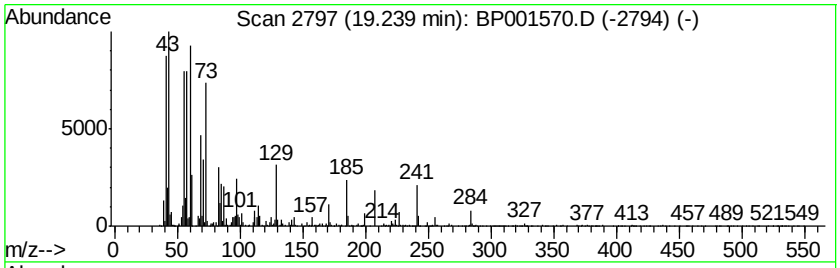
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

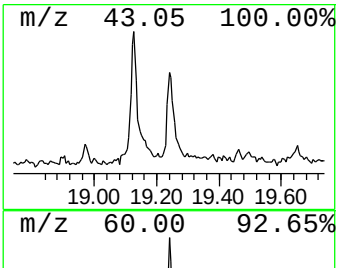
****

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	2.12 ng	80512	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

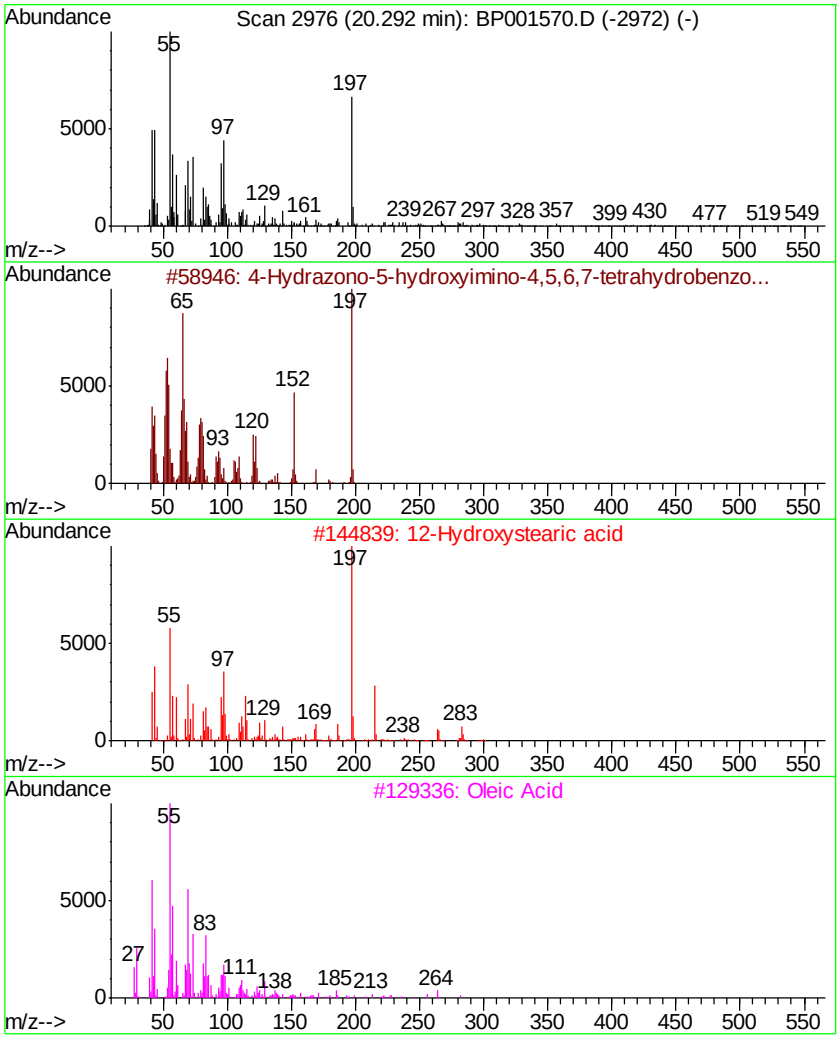
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

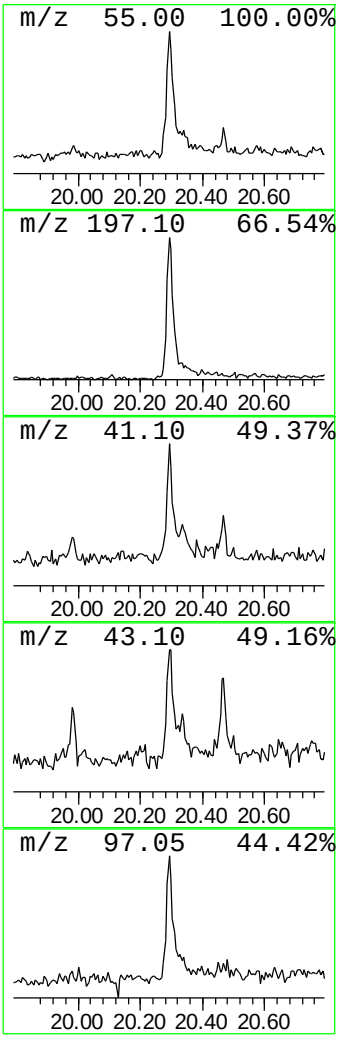
****

Peak Number 8 4-Hydrazono-5-hydroxyimino-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	2.15 ng	81597	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	91
2	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	55
3	Oleic Acid	282	C18H34O2	000112-80-1	41
4	3-Oxo-1-cyclohexene-1-carboxylic...	212	C10H16O3Si	1000332-58-2	25
5	Benzenamine, 2,3,4-trichloro-	195	C6H4Cl3N	000634-67-3	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

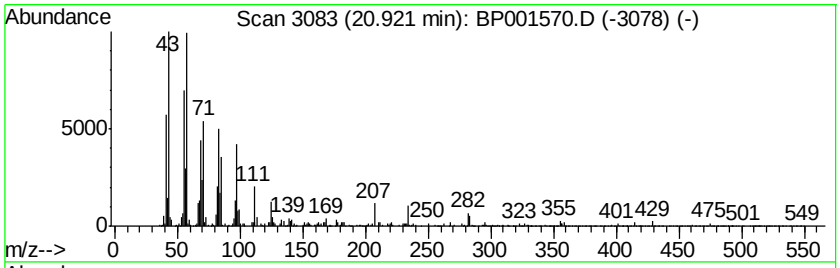
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

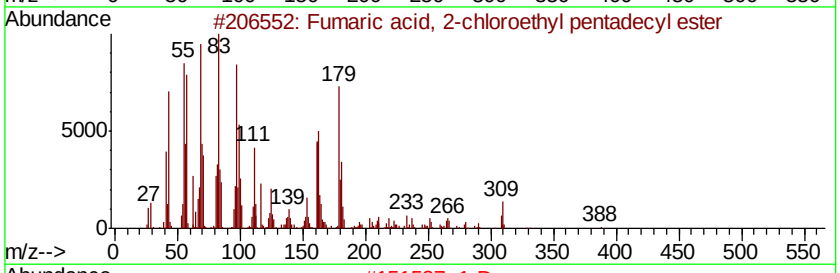
****

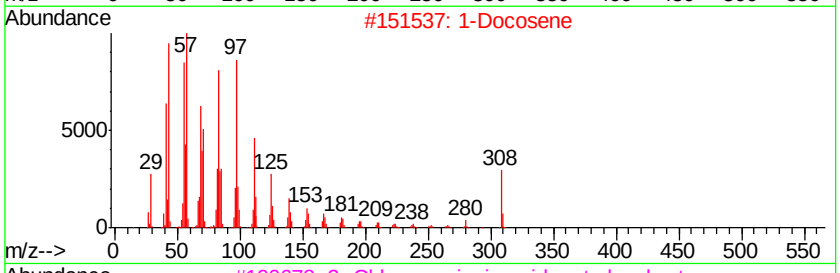
Peak Number 9 Fumaric acid, 2-chloroethyl... Concentration Rank 7

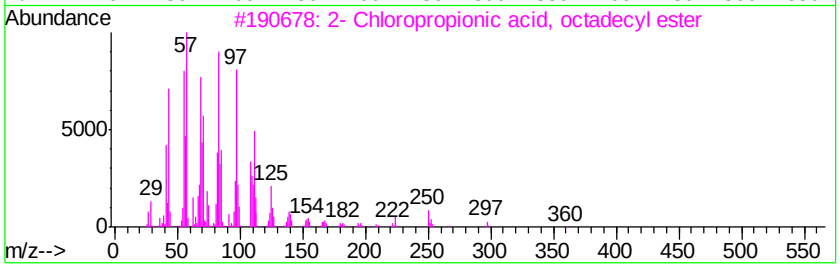
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	3.09 ng	117589	Chrysene-d12	21.16

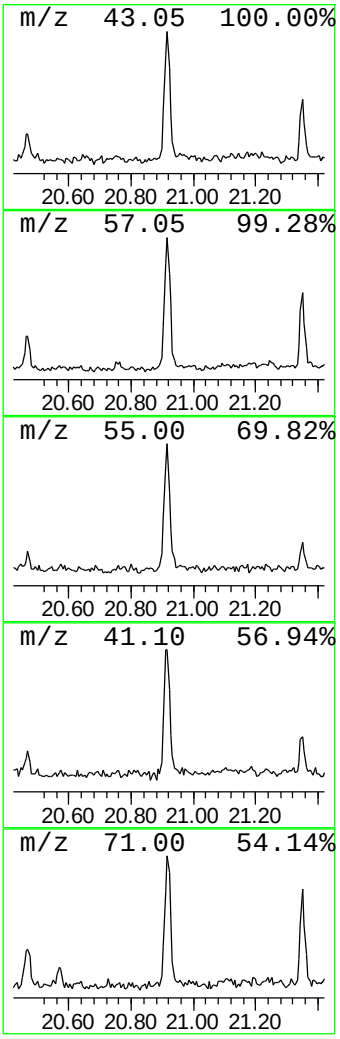
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloroethyl pent...	388	C21H37ClO4	1000330-62-1	98
2	1-Docosene	308	C22H44	001599-67-3	97
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	1-Hexacosene	364	C26H52	018835-33-1	91











Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

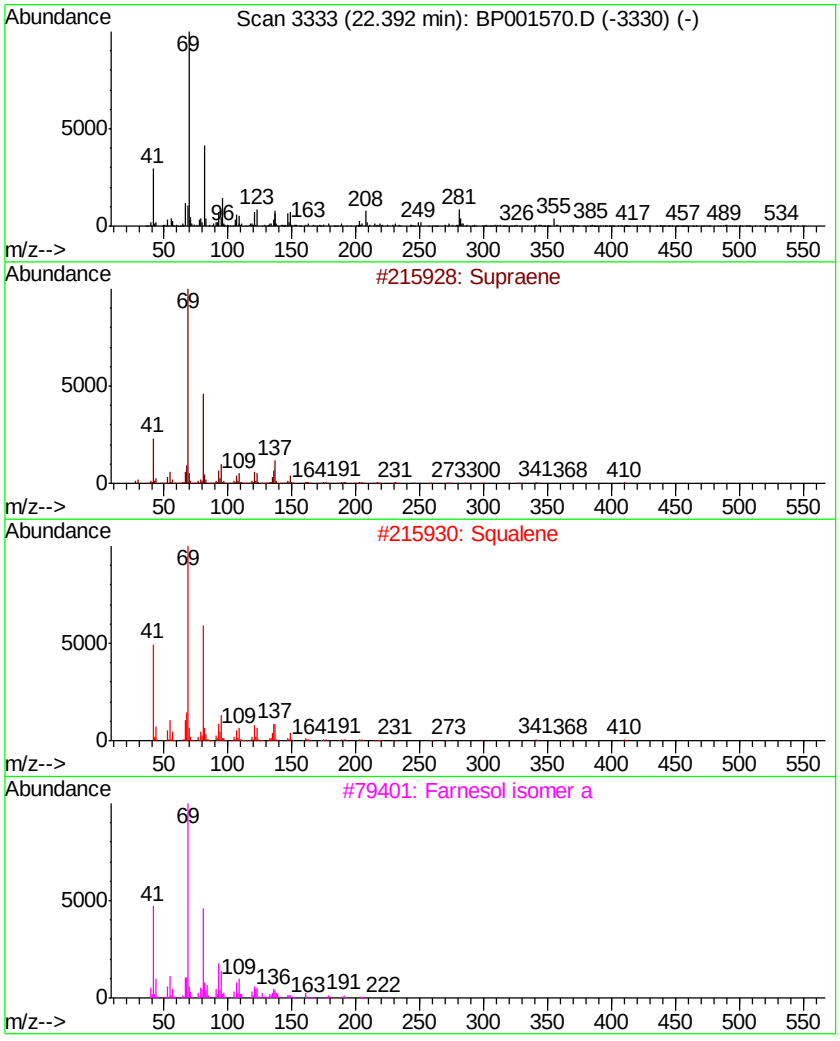
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

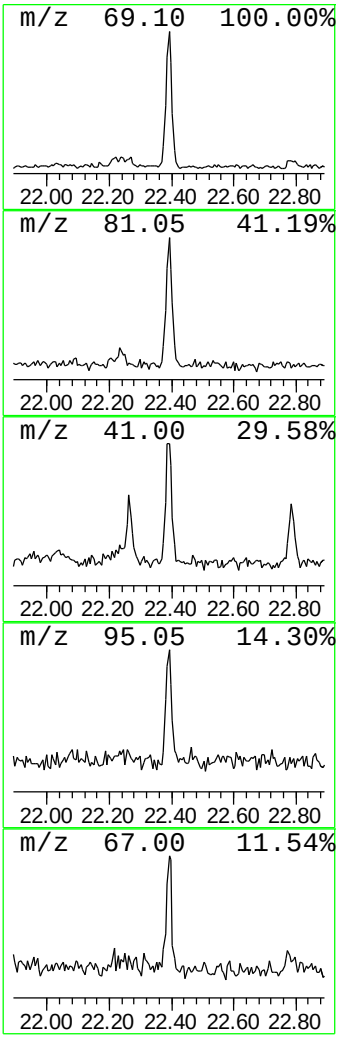
****

Peak Number 10 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	2.02 ng	67354	Perylene-d12	23.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	68
2	Squalene	410	C30H50	000111-02-4	64
3	Farnesol isomer a	222	C15H26O	1000108-92-4	59
4	6-Bromohexanoic acid, tridec-2-y...	372	C19H33BrO2	1000299-29-5	59
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP010820\
Data File : BP001570.D
Acq On : 09 Jan 2020 01:21
Operator : JU
Sample : L1051-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4F-(22-24)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.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-methoxy...	2.98	17.7	ng	210641	1	7.66	237627	20.0
2-Pentanone, 4-hy...	4.83	20.6	ng	245220	1	7.66	237627	20.0
unknown7.20	7.20	116.8	ng	1388310	1	7.66	237627	20.0
n-Hexadecanoic acid	18.00	4.9	ng	153030	4	17.06	619583	20.0
Octadecanoic acid	19.24	2.1	ng	80512	5	21.16	760695	20.0
4-Hydrazono-5-hyd...	20.29	2.1	ng	81597	5	21.16	760695	20.0
Fumaric acid, 2-c...	20.92	3.1	ng	117589	5	21.16	760695	20.0
Supraene	22.39	2.0	ng	67354	6	23.42	665436	20.0