LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016349.D
Acq On : 14 Aug 2018 11:47
Operator : SJ/JU
Sample : J4430-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : UST-E

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_M\METHODS\8270-BM072318.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	5.175	315	321	331	rBV	76241	117324	9.36%	1.357%
2	5.645	396	401	421	rBB	499607	784832	62.61%	9.079%
3	7.287	674	680	695	rBV	498807	799686	63.79%	9.251%
4	7.645	735	741	754	rBB	580970	908943	72.51%	10.515%
5	8.116	816	821	830	rBB	117007	183695	14.65%	2.125%
6	8.439	869	876	886	rBB	402310	660940	52.73%	7.646%
7	9.304	1017	1023	1034	rBV	299459	500137	39.90%	5.786%
8	10.933	1294	1300	1308	rBV	119861	204606	16.32%	2.367%
9	13.368	1708	1714	1721	rBV	602773	867201	69.18%	10.032%
10	14.210	1852	1857	1865	rBB	38443	51537	4.11%	0.596%
11	14.751	1943	1949	1956	rBB2	147462	224969	17.95%	2.602%
12	16.239	2197	2202	2212	rVB	560284	791913	63.17%	9.161%
13	17.492	2406	2415	2422	rBV	173079	249861	19.93%	2.890%
14	18.339	2554	2559	2570	rBV	57331	83524	6.66%	0.966%
15	19.597	2769	2773	2777	rBV2	33251	39905	3.18%	0.462%
16	20.068	2848	2853	2858	rBV	1096320	1253553	100.00%	14.501%
17	20.827	2979	2982	2987	rVB6	12967	15396	1.23%	0.178%
18	21.291	3056	3061	3068	rBV6	44341	82766	6.60%	0.957%
19	21.621	3112	3117	3123	rBV2	279758	352642	28.13%	4.079%
20	21.715	3130	3133	3138	rBV	23252	24956	1.99%	0.289%
21	22.162	3206	3209	3213	rVB3	22246	25752	2.05%	0.298%
22	22.633	3286	3289	3292	rVB3	32477	36961	2.95%	0.428%
23	23.150	3374	3377	3382	rVB3	33673	47621	3.80%	0.551%
24	23.950	3507	3513	3522	rVB	182913	335742	26.78%	3.884%

Sum of corrected areas: 8644462

LSC Report - Integrated Chromatogram

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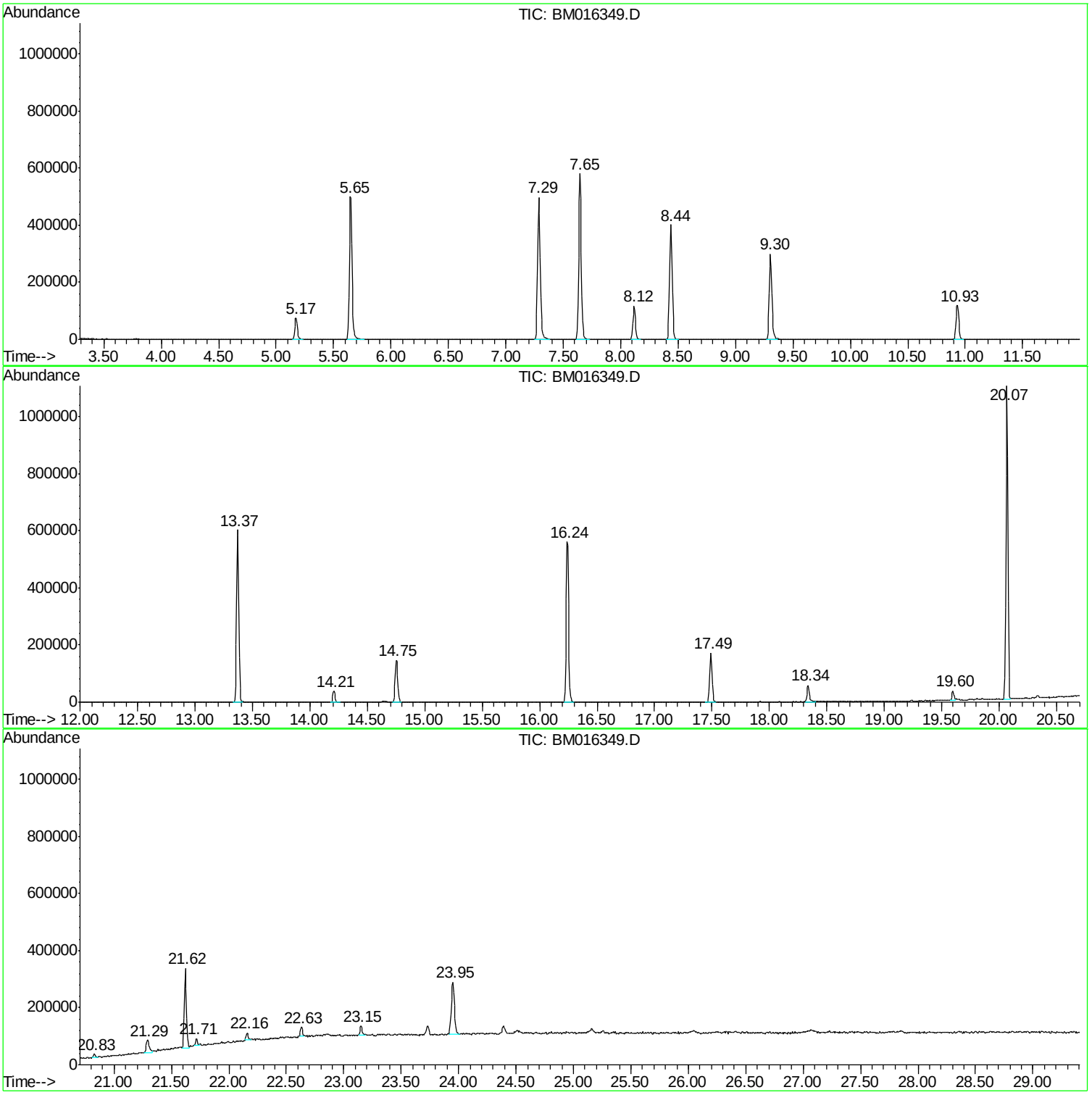
Sample : J4430-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : UST-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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ClientSampleId : UST-E

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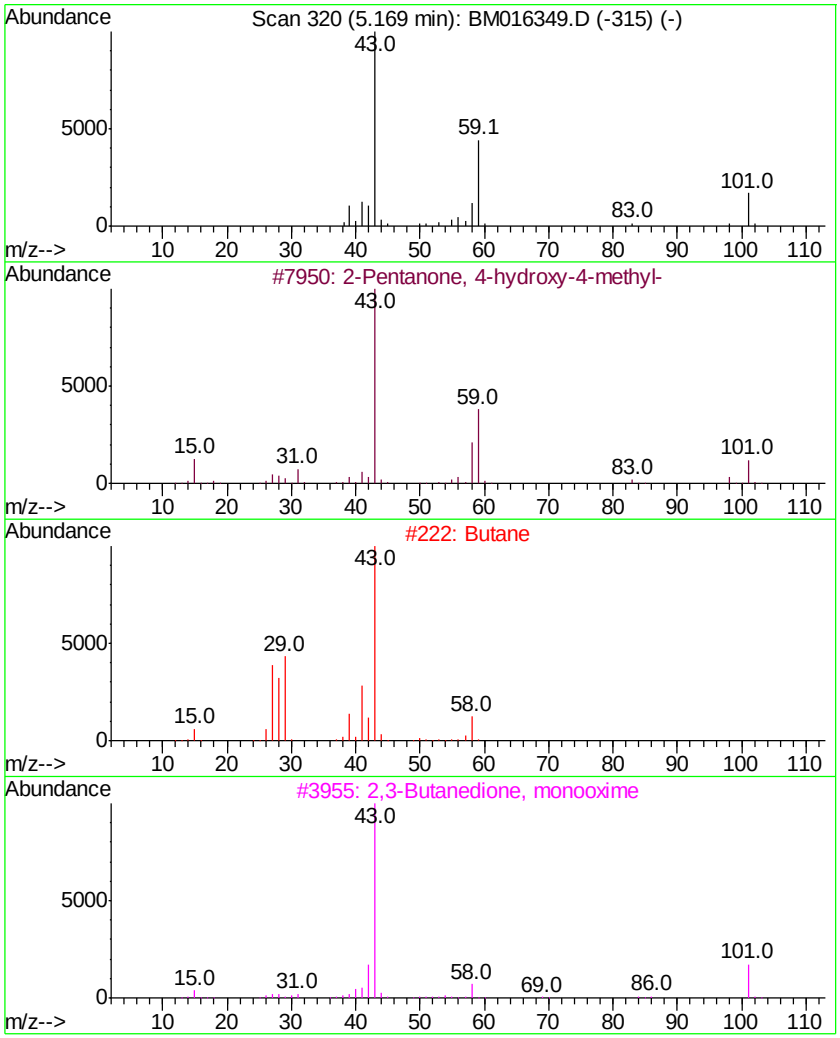
TIC Integration Parameters: LSCINT.P

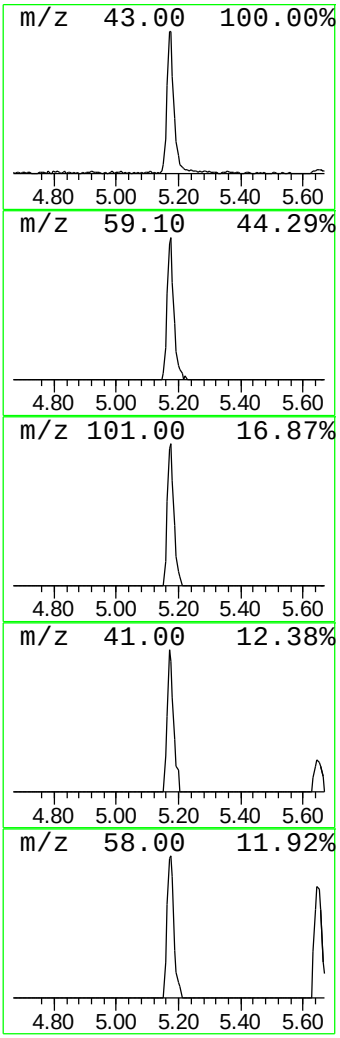
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.77 ng	117324	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Butane	58	C4H10	000106-97-8	27
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : UST-E

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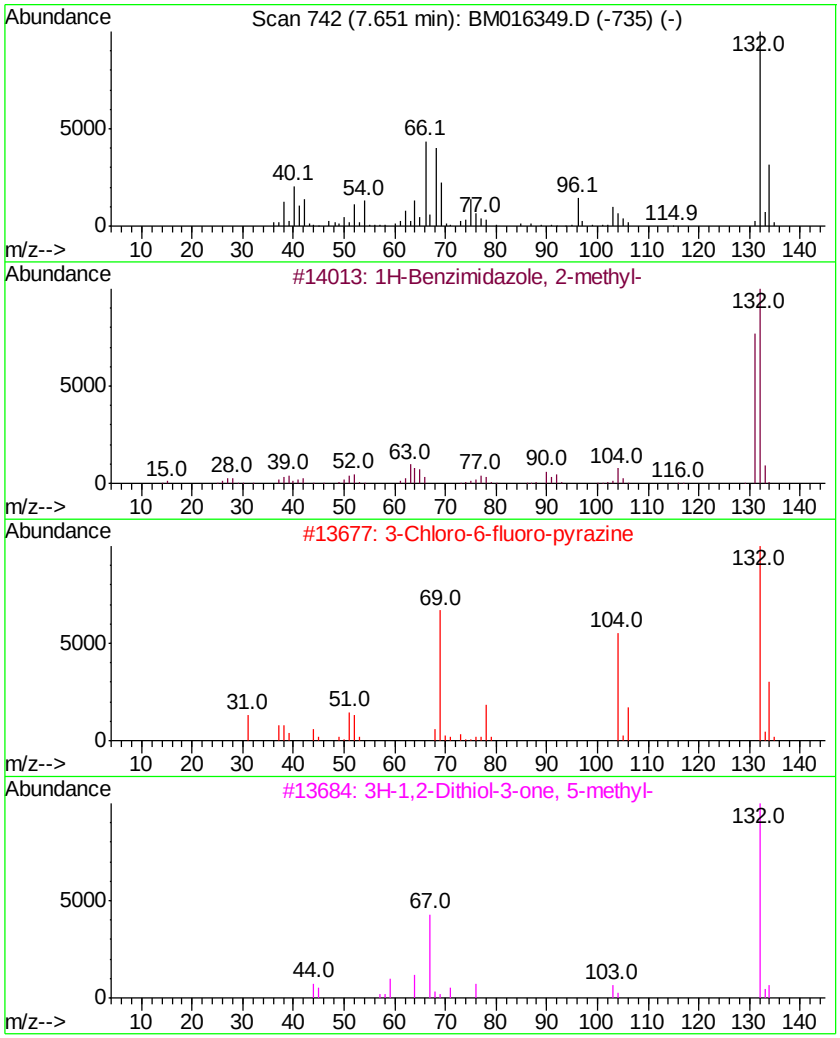
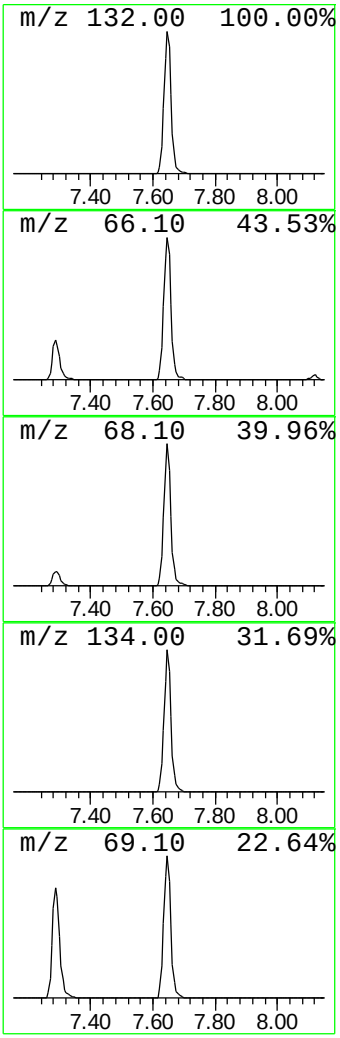
****

Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	98.96 ng	908943	1,4-Dichlorobenzene-d4	8.12

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





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016349.D
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Sample : J4430-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : UST-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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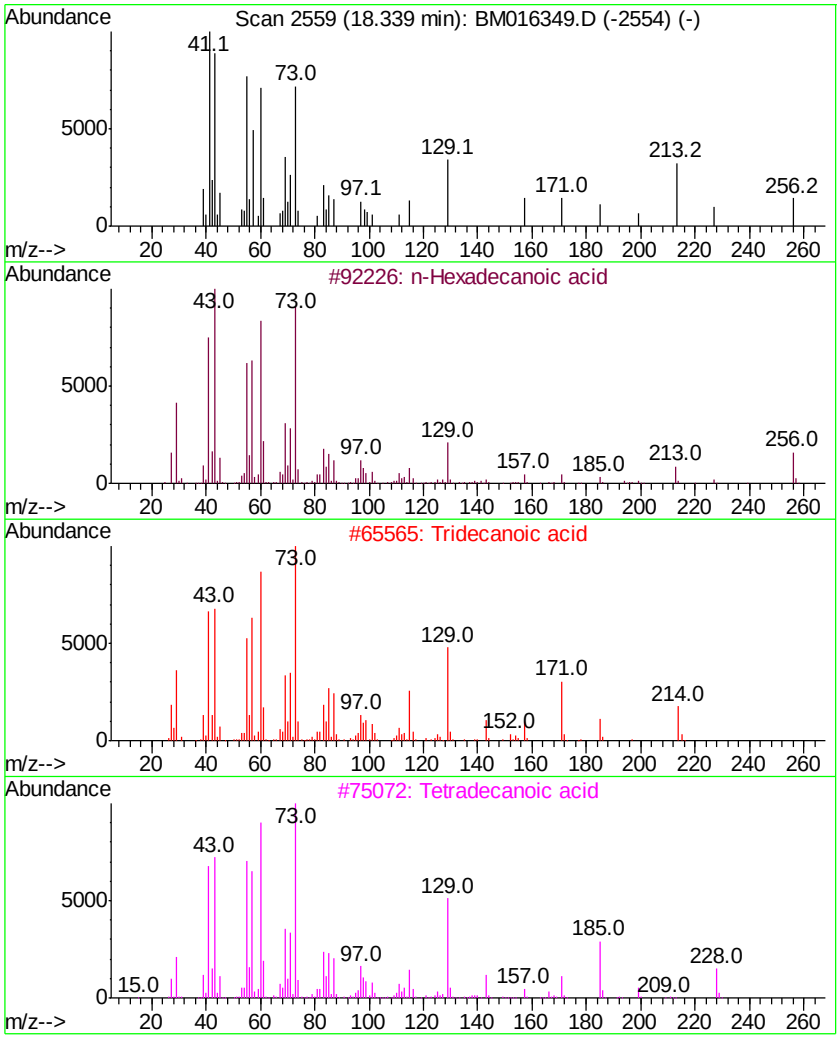
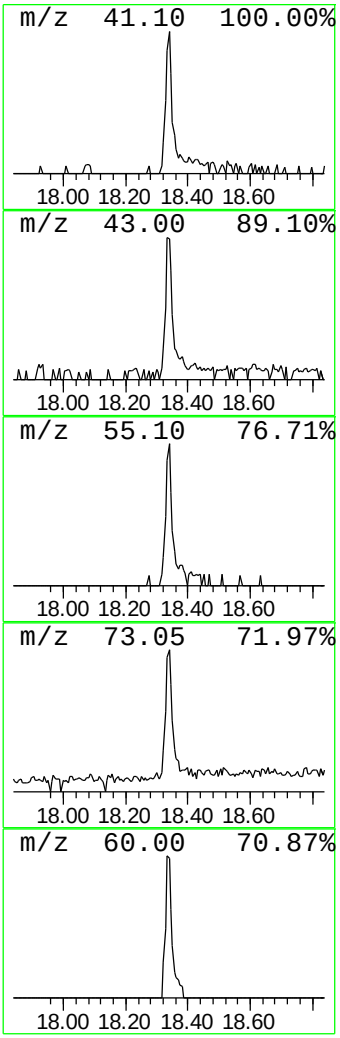
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	6.69 ng	83524	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Sample : J4430-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : UST-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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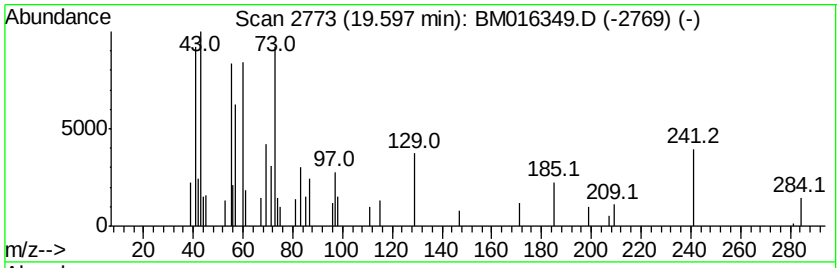
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

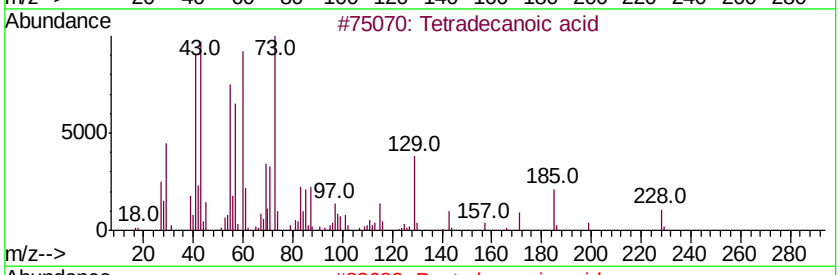
****

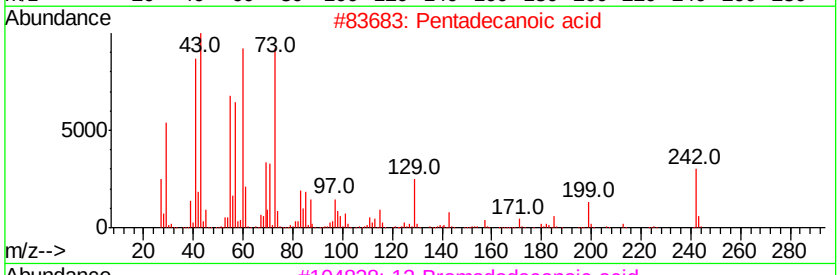
Peak Number 5 Tetradecanoic acid Concentration Rank 7

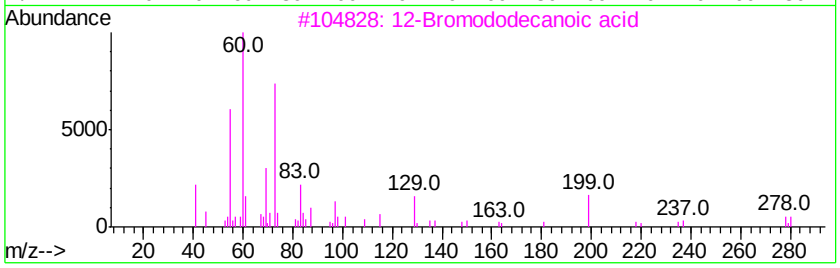
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.26 ng	39905	Chrysene-d12	21.62

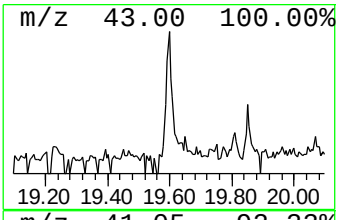
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
3	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	38
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	37

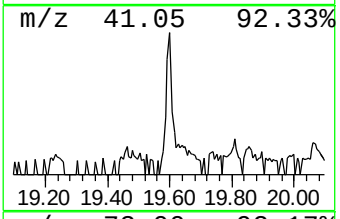


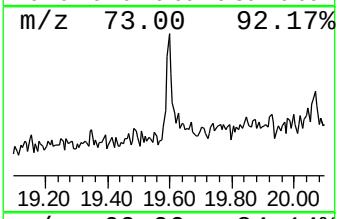


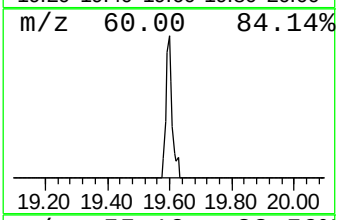


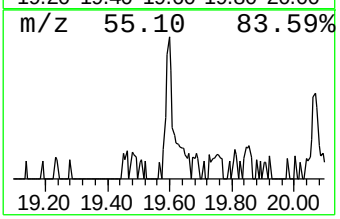












Library Search Compound Report

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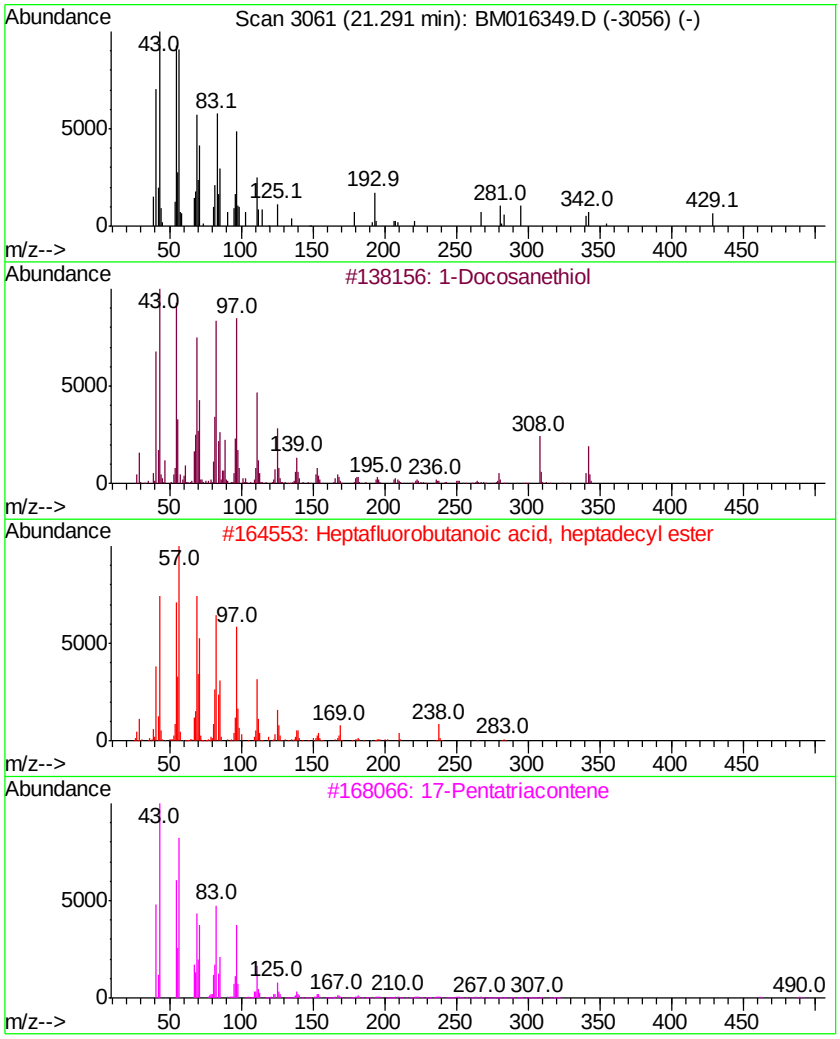
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

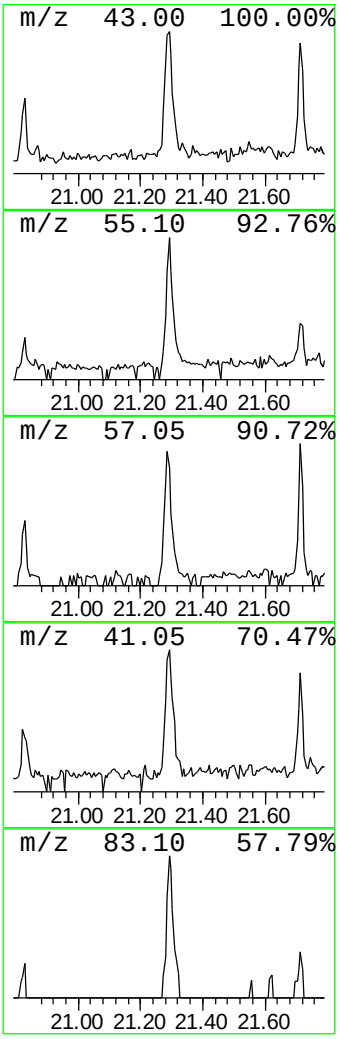
****

Peak Number 6 1-Docosanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.69 ng	82766	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	94
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
3	17-Pentatriacontene	491	C35H70	006971-40-0	81
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	74
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	74





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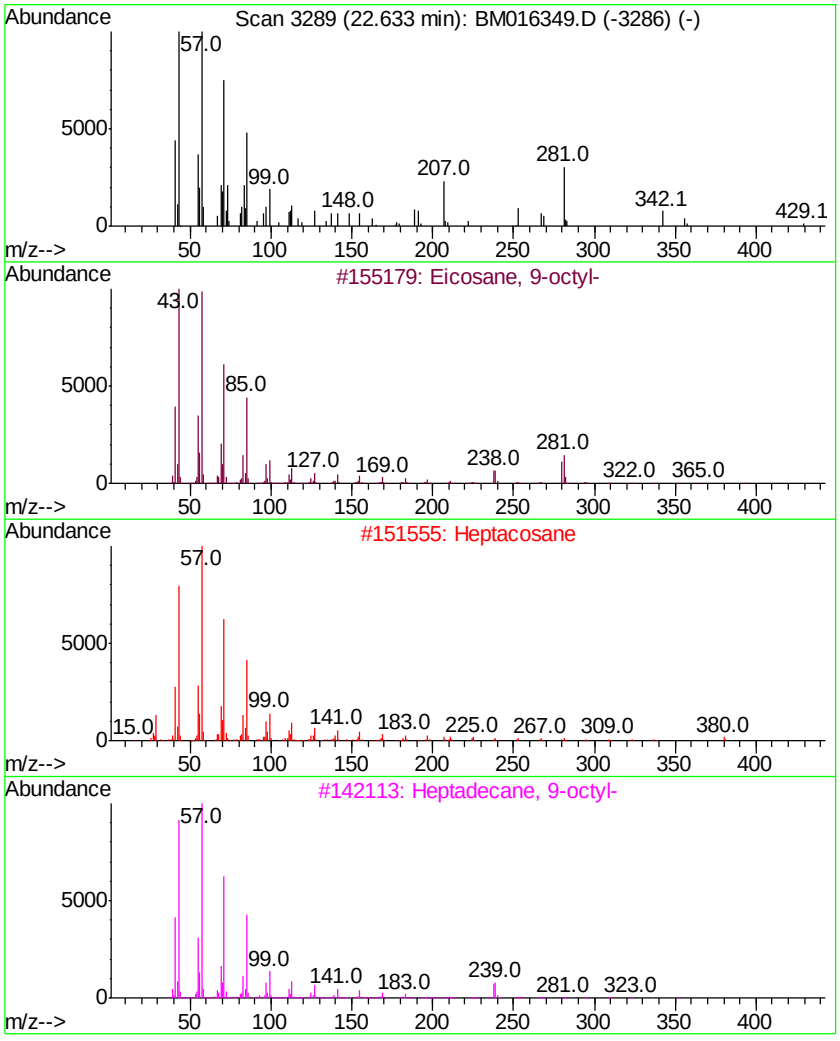
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

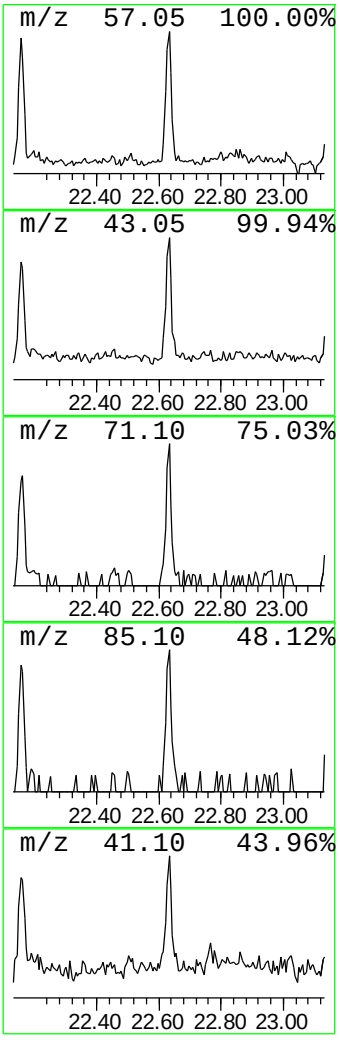
****

Peak Number 7 Eicosane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.10 ng	36961	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 9-octyl-	394	C28H58	013475-77-9	58
2	Heptacosane	380	C27H56	000593-49-7	53
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	53
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	53





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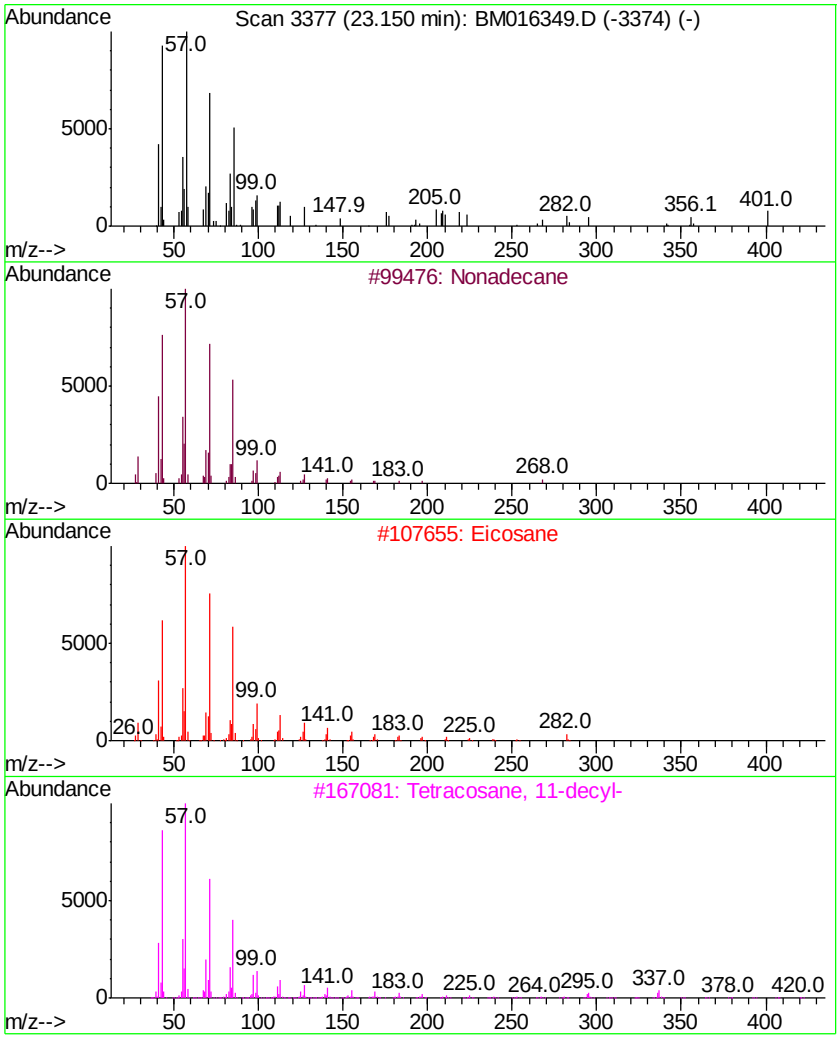
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

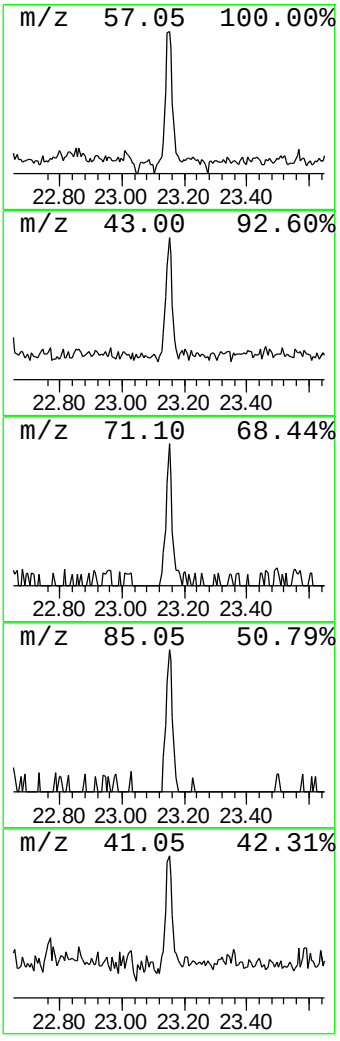
****

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	2.84 ng	47621	Perylene-d12	23.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Eicosane	282	C20H42	000112-95-8	81
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	72
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	72
5	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	64





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	12.8	ng	117324	1	8.12	183695	20.0
unknown7.65	7.65	99.0	ng	908943	1	8.12	183695	20.0
n-Hexadecanoic acid	18.34	6.7	ng	83524	4	17.49	249861	20.0
Tetradecanoic acid	19.60	2.3	ng	39905	5	21.62	352642	20.0
1-Docosanethiol	21.29	4.7	ng	82766	5	21.62	352642	20.0
Eicosane, 9-octyl-	22.63	2.1	ng	36961	5	21.62	352642	20.0
Nonadecane	23.15	2.8	ng	47621	6	23.95	335742	20.0