LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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	5.169	314	320	330	rBV	59214	88909	3.14%	0.554%
2	5.645	396	401	414	rBV	427247	660411	23.31%	4.112%
3	7.287	674	680	695	rBV	229878	395236	13.95%	2.461%
4	7.645	734	741	757	rBV	999384	1562951	55.16%	9.733%
5	8.116	815	821	829	rBV	181744	294226	10.38%	1.832%
6	8.434	869	875	888	rBB	960454	1537025	54.24%	9.571%
7	9.304	1016	1023	1037	rBV	722255	1186214	41.86%	7.387%
8	10.333	1192	1198	1205	rBB2	27630	41338	1.46%	0.257%
9	10.927	1293	1299	1304	rBV	214768	355201	12.54%	2.212%
10	10.980	1304	1308	1317	rVB	102456	172790	6.10%	1.076%
11	13.374	1708	1715	1721	rBV	1668463	2415223	85.24%	15.040%
12	14.204	1851	1856	1862	rBV	43506	60506	2.14%	0.377%
13	14.751	1943	1949	1956	rBV2	263767	395709	13.97%	2.464%
14	14.815	1956	1960	1965	rVB2	21519	30342	1.07%	0.189%
15	16.245	2196	2203	2212	rBV	1360383	1838655	64.89%	11.450%
16	17.486	2409	2414	2419	rBV2	306151	427607	15.09%	2.663%
17	17.903	2481	2485	2489	rBV	34141	49484	1.75%	0.308%
18	18.339	2554	2559	2568	rBV	104506	157471	5.56%	0.981%
19	19.598	2769	2773	2780	rBV2	64199	93967	3.32%	0.585%
20	19.892	2820	2823	2829	rVB3	19622	29962	1.06%	0.187%
21	20.068	2848	2853	2862	rBV	2514441	2833494	100.00%	17.645%
22	20.333	2895	2898	2903	rBV3	24915	31771	1.12%	0.198%
23	20.827	2978	2982	2985	rBV	46208	47598	1.68%	0.296%
24	21.286	3056	3060	3070	rBV4	150430	265672	9.38%	1.654%
25	21.621	3112	3117	3123	rVB	335903	419696	14.81%	2.614%
26	21.715	3130	3133	3137	rVB	52029	53847	1.90%	0.335%
27	22.156	3205	3208	3212	rBV	54727	61757	2.18%	0.385%
28	22.633	3286	3289	3293	rVB	47213	55898	1.97%	0.348%
29	23.150	3374	3377	3382	rVB3	49149	65968	2.33%	0.411%
30	23.950	3508	3513	3522	rVB2	225314	429745	15.17%	2.676%

Sum of corrected areas: 16058673

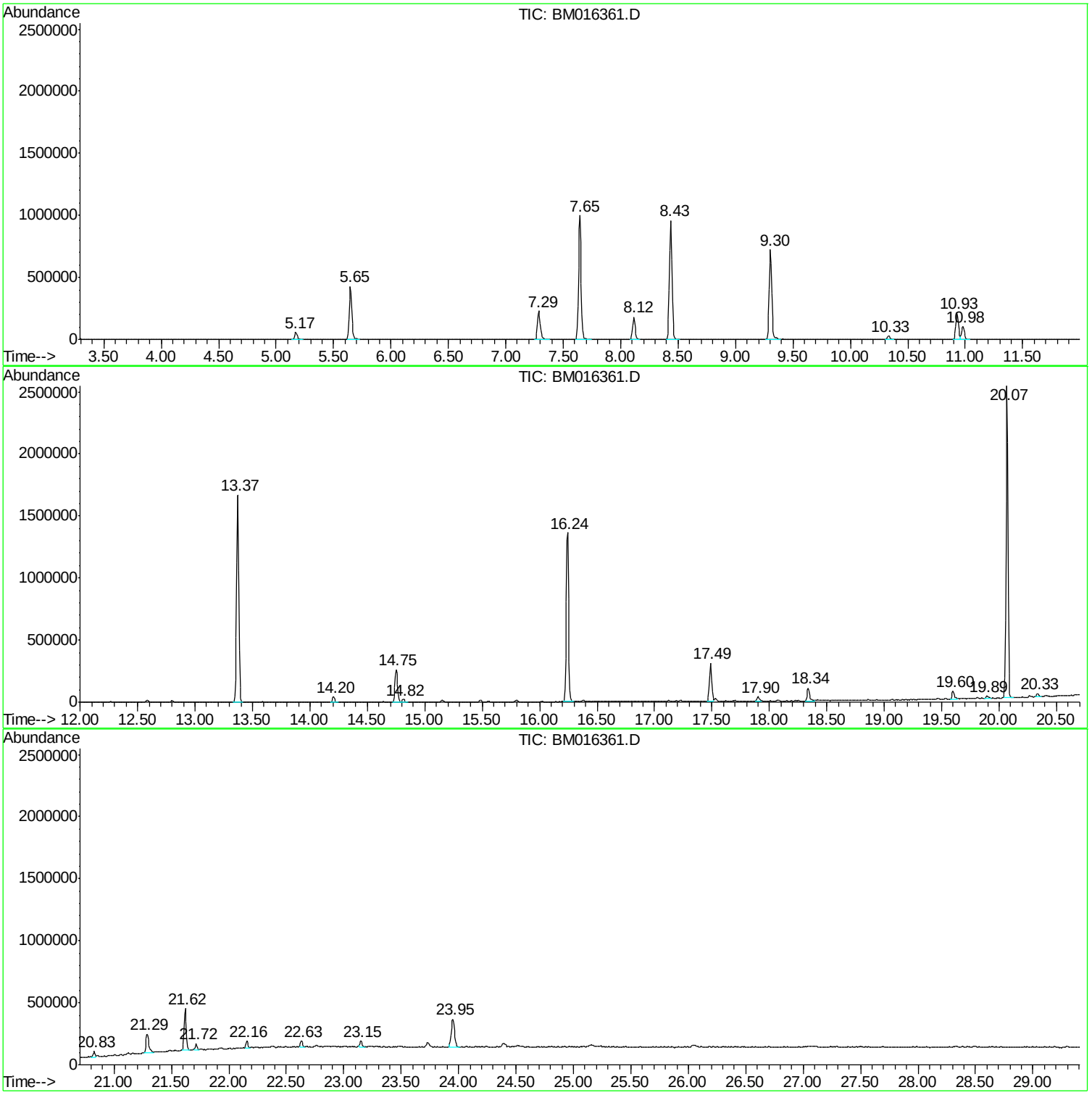
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
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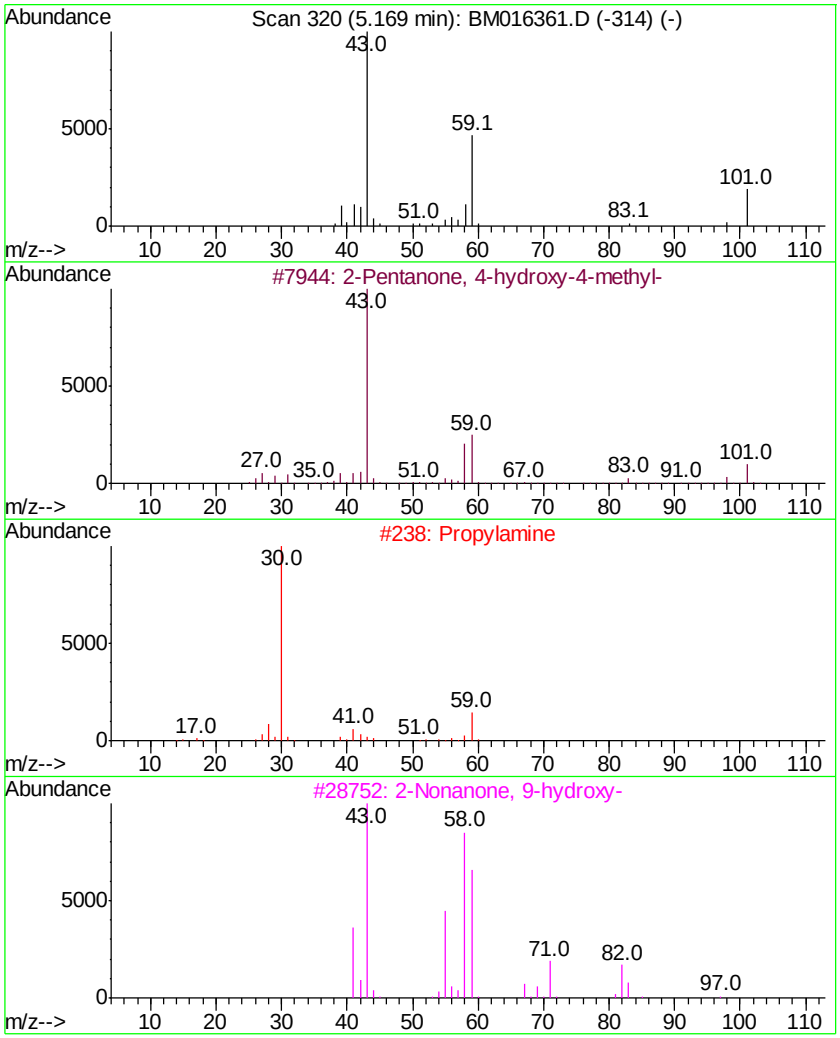
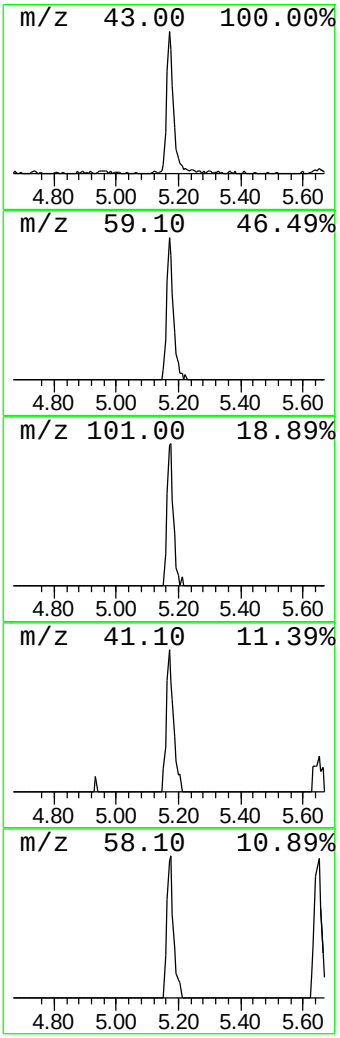
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	6.04 ng	88909	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	72
2	Propylamine	59	C3H9N	000107-10-8	42
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
5	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	32





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Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

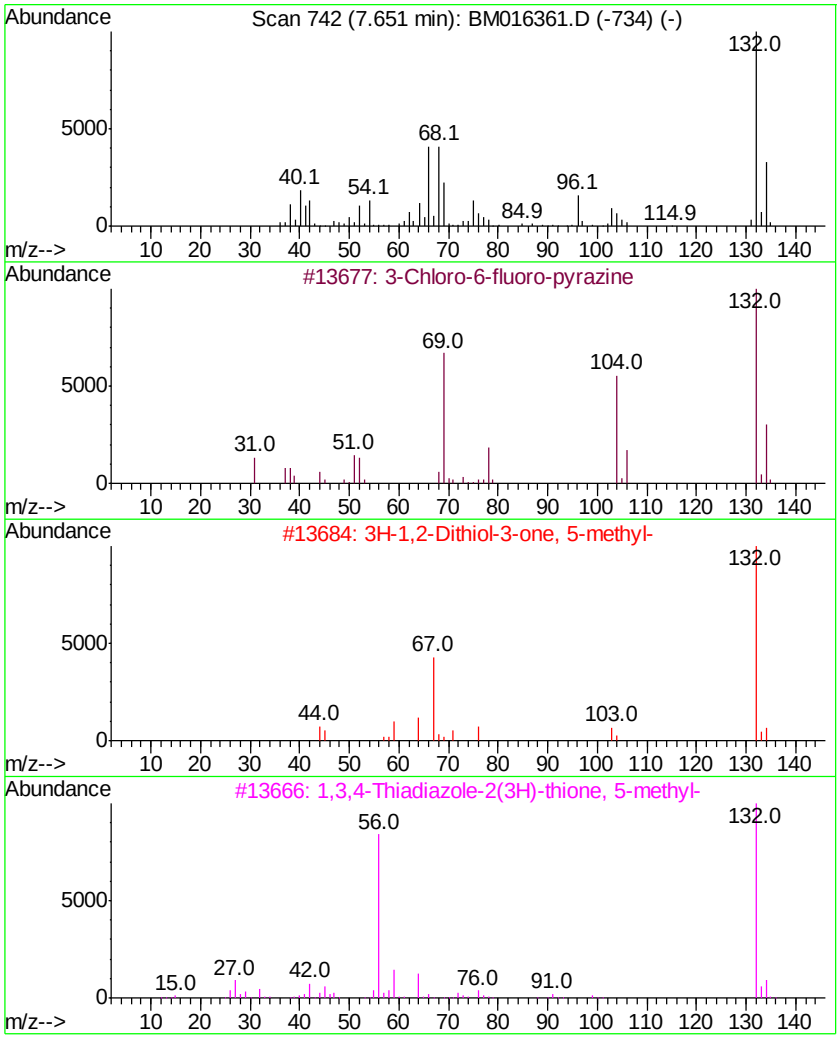
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

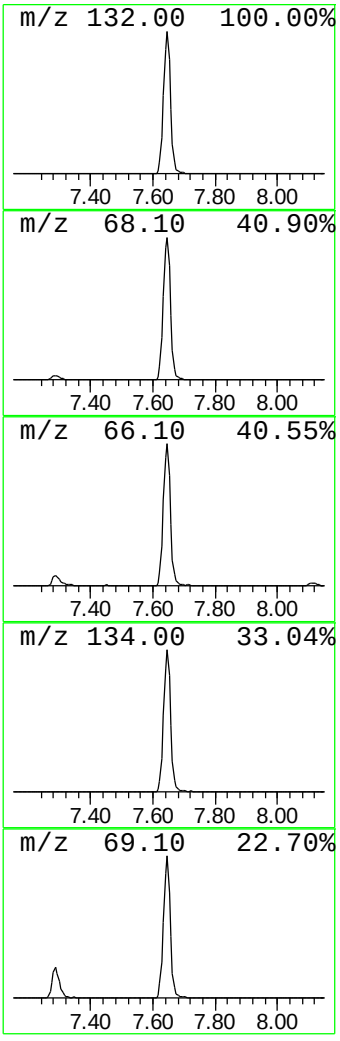
****

Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	106.24 ng	1562950	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : GMW-11

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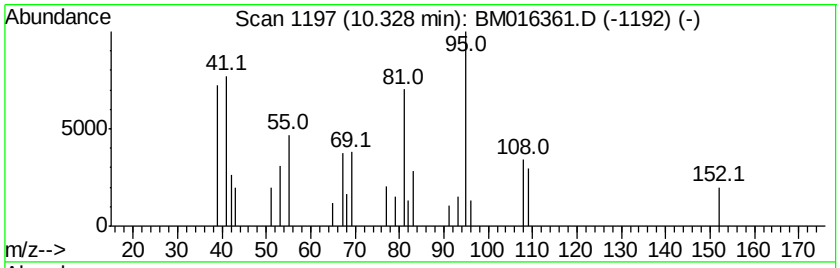
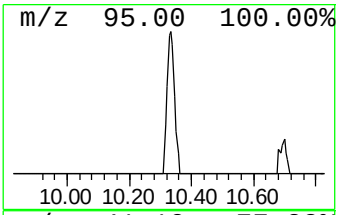
****

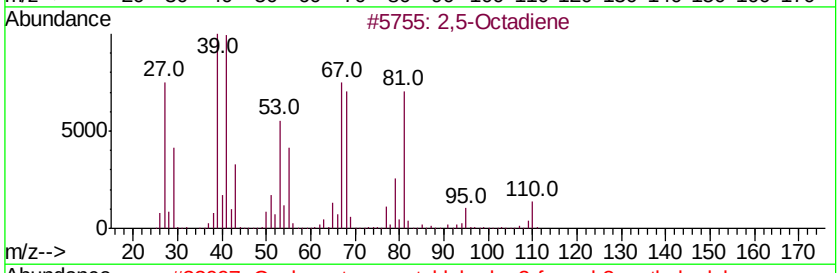
Peak Number 4 2,5-Octadiene Concentration Rank 11

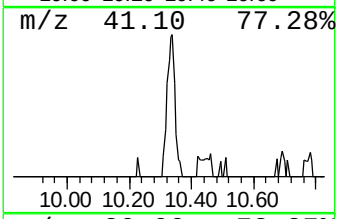
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.33 ng	41338	Naphthalene-d8	10.93

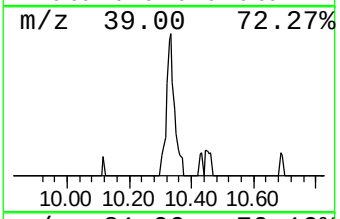
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Octadiene	110	C8H14	063216-69-3	68
2	Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	59
3	2,4-Hexadienal, (E,E)-	96	C6H8O	000142-83-6	53
4	Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	50
5	2-Octyne	110	C8H14	002809-67-8	43

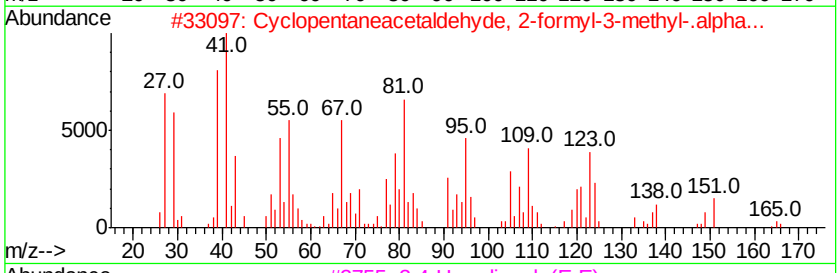


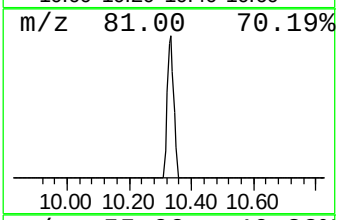


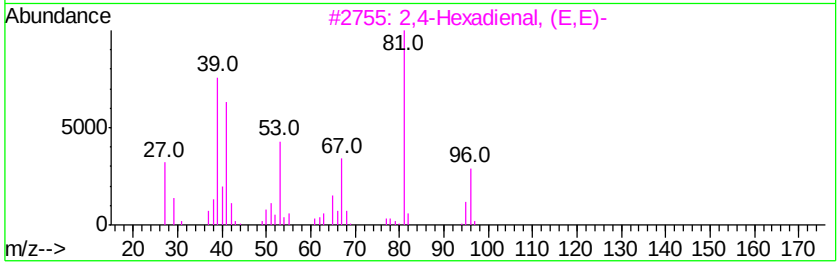


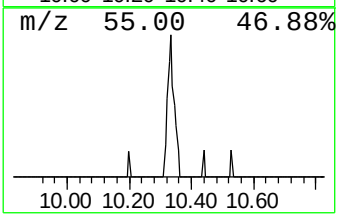












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

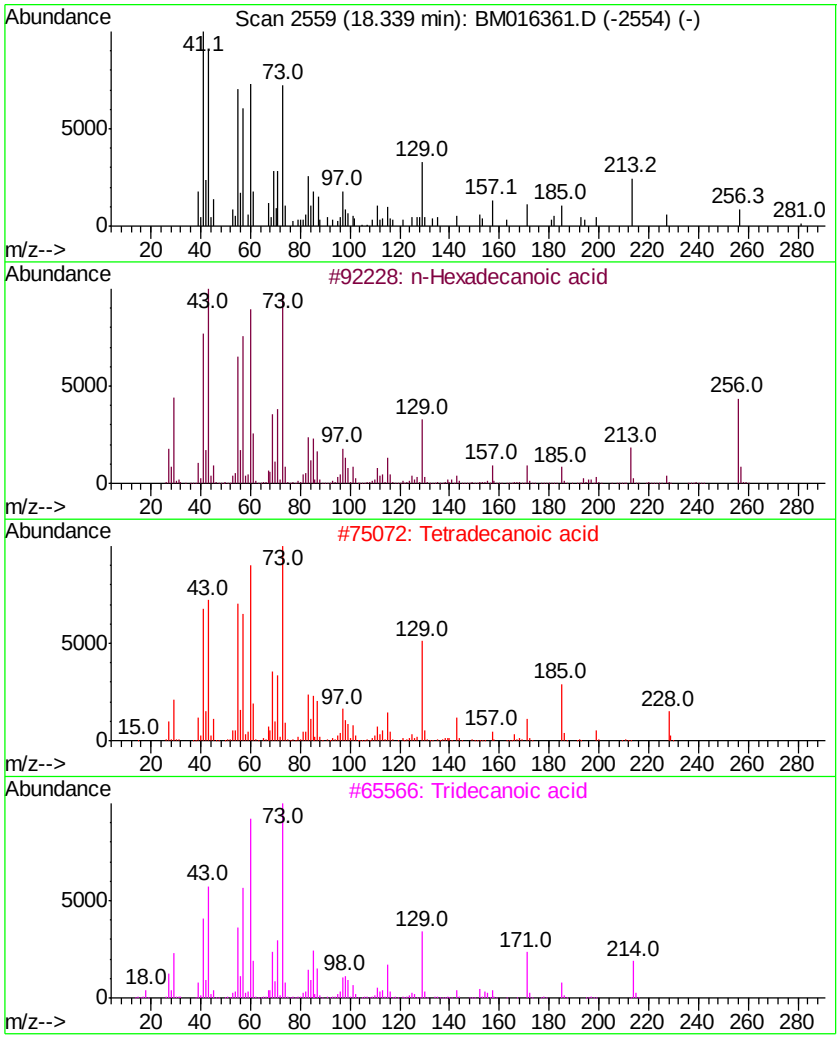
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

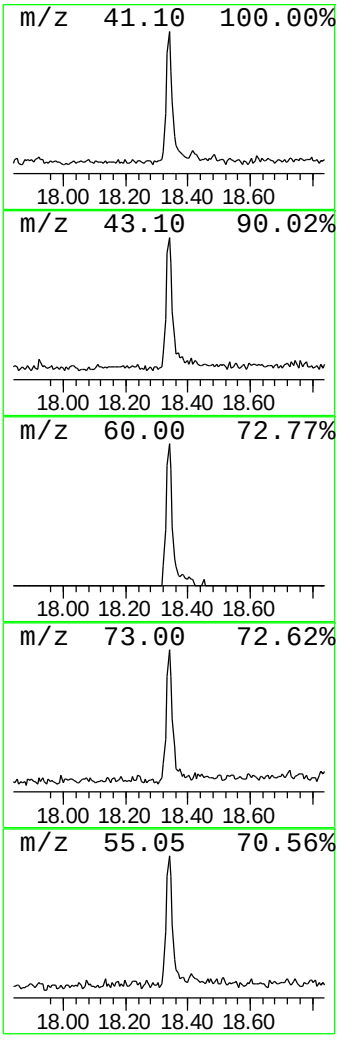
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	7.37 ng	157471	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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
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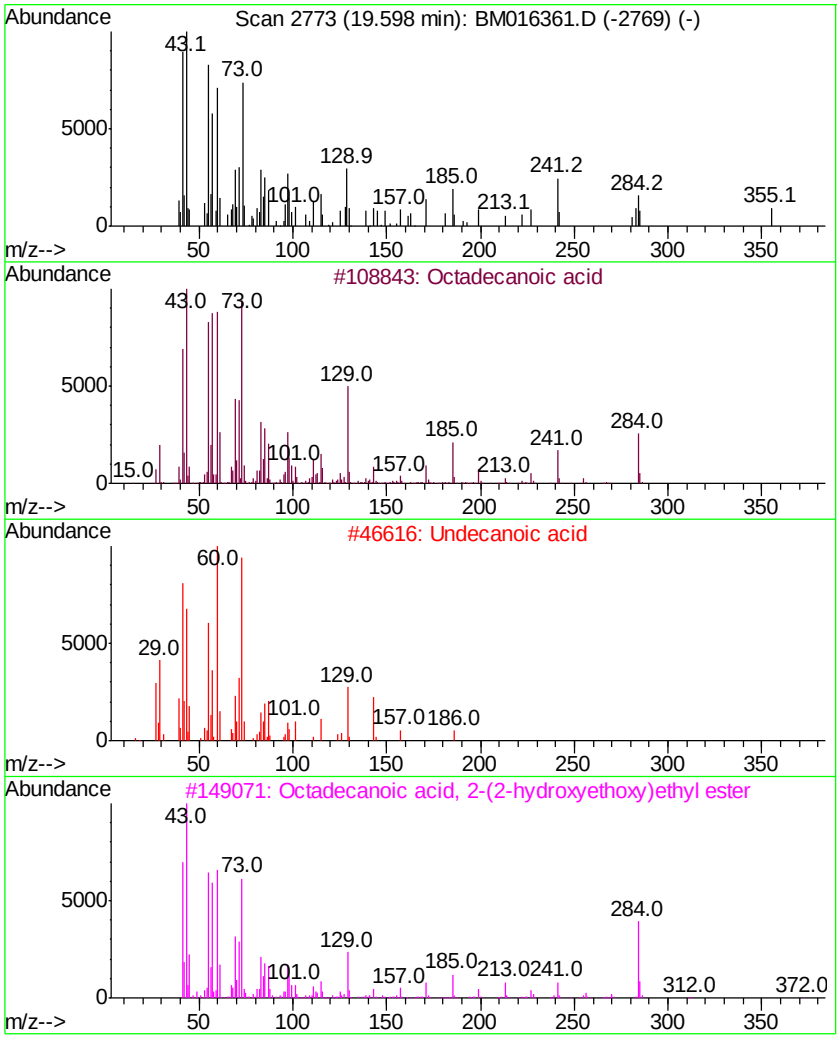
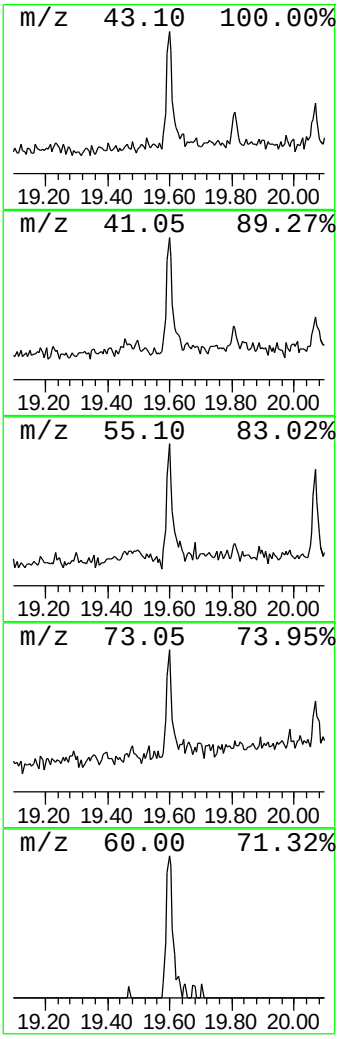
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	4.48 ng	93967	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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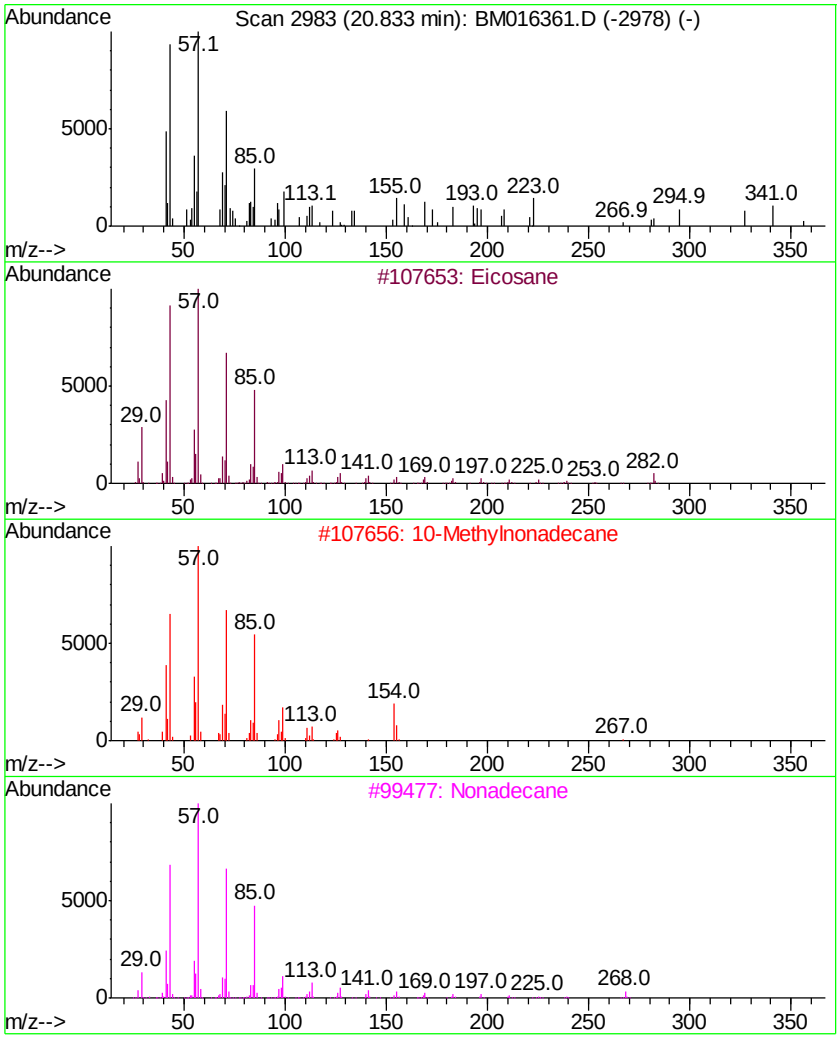
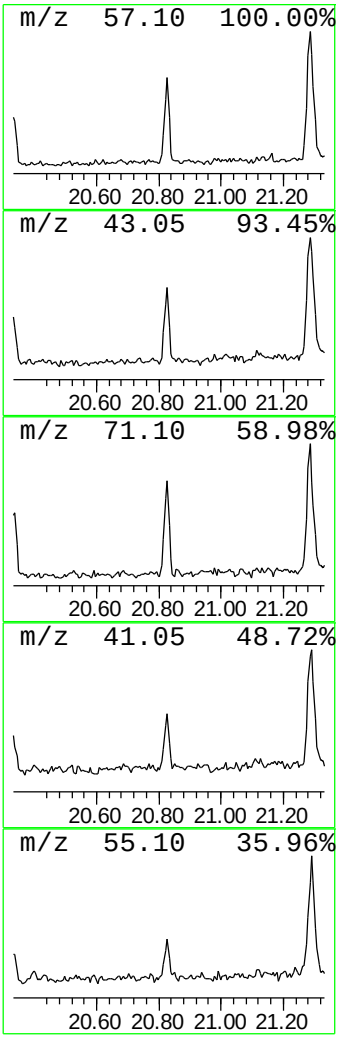
****

Peak Number 7 10-Methylnonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.83	2.27 ng	47598	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	10-Methylnonadecane	282	C20H42	056862-62-5	81
3	Nonadecane	268	C19H40	000629-92-5	81
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
5	Octacosane	394	C28H58	000630-02-4	74





Library Search Compound Report

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Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

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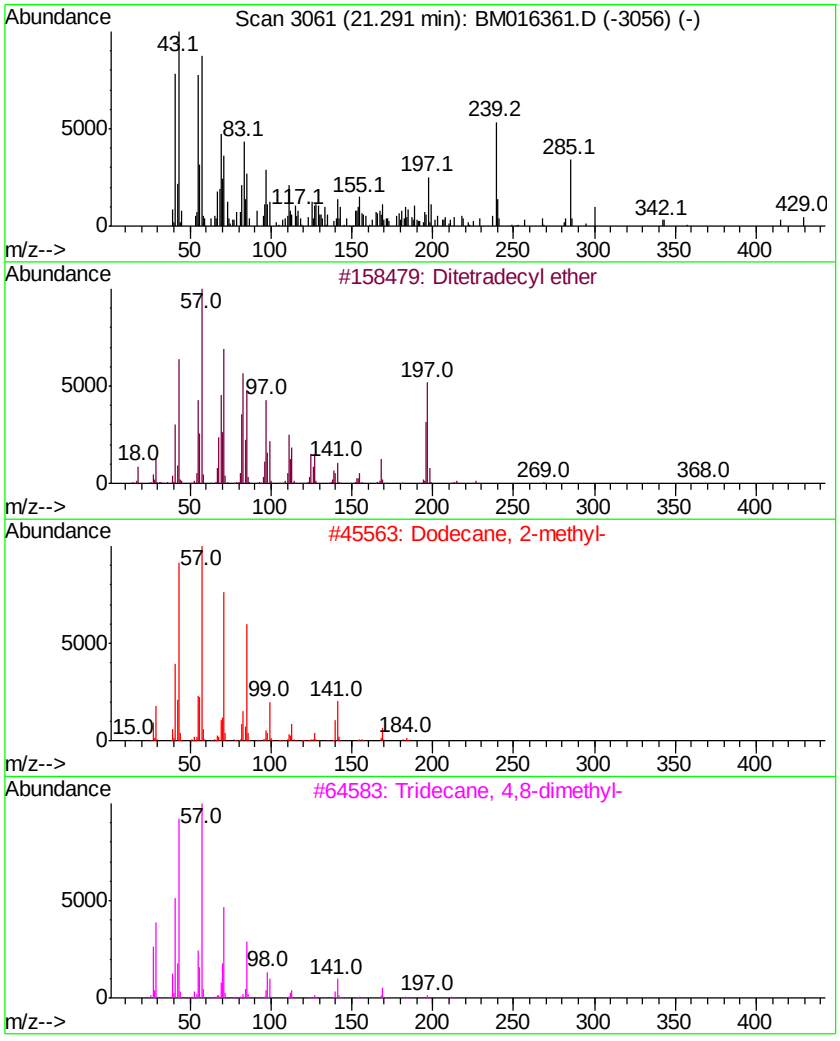
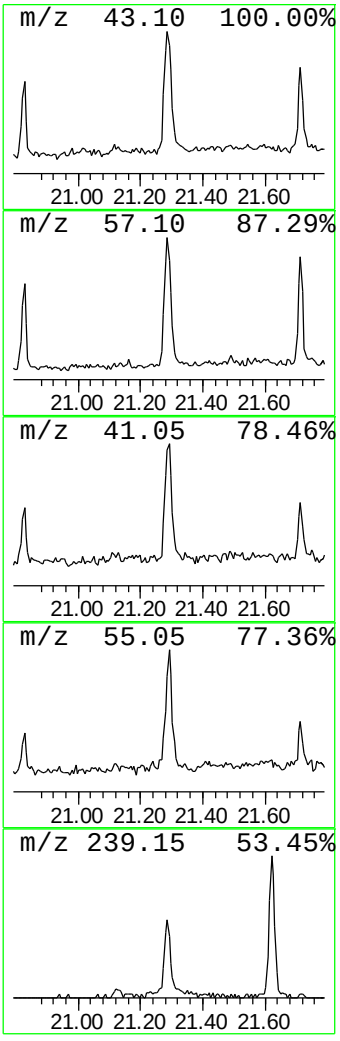
Peak Number 8 unknown21.29 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	12.66 ng	265672	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ditetradecyl ether	410	C28H58O	005412-98-6	43
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	42
3	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	30
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	27
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	27





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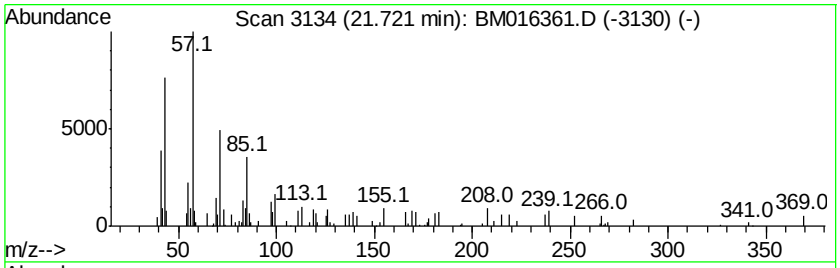
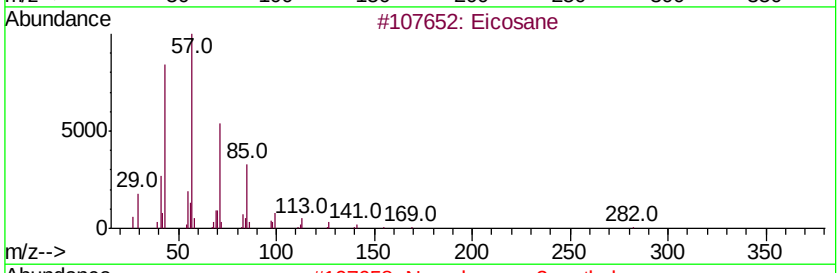
****

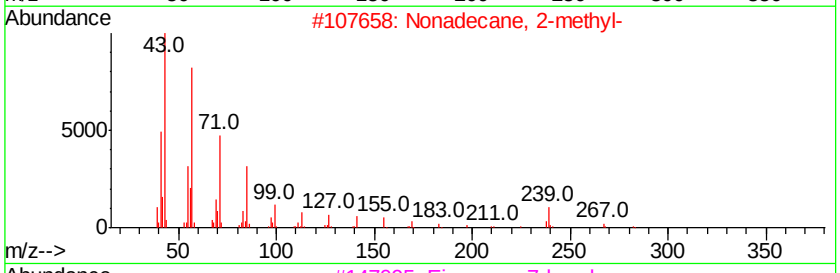
Peak Number 9 Eicosane Concentration Rank 10

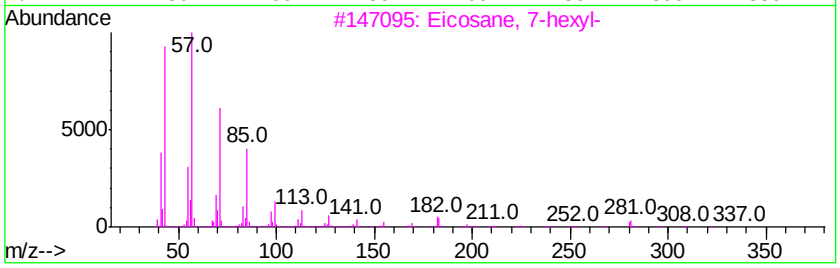
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.57 ng	53847	Chrysene-d12	21.62

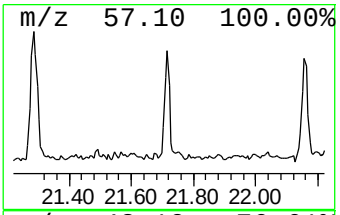
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	89
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	81
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	74
5	Hexatriacontane	507	C36H74	000630-06-8	74

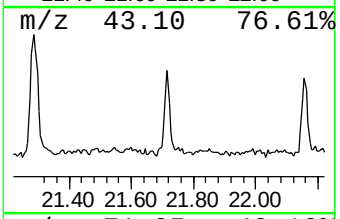


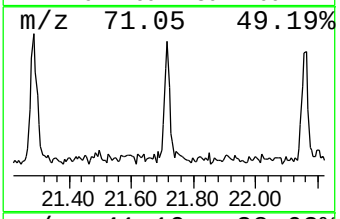


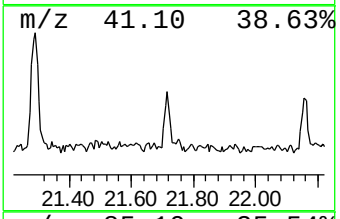


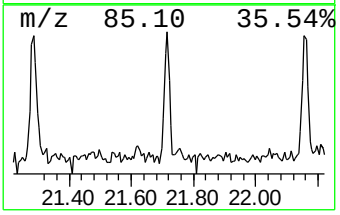












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GMW-11

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

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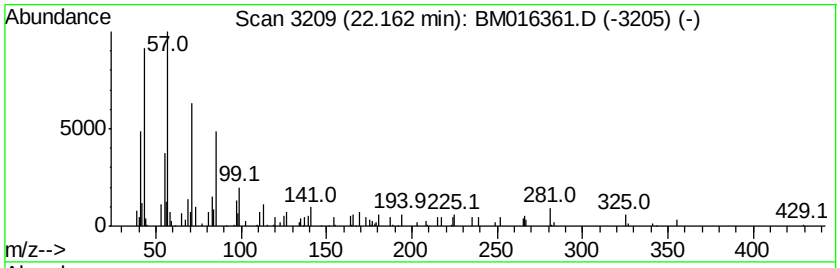
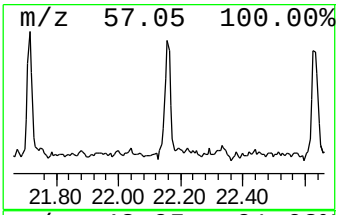
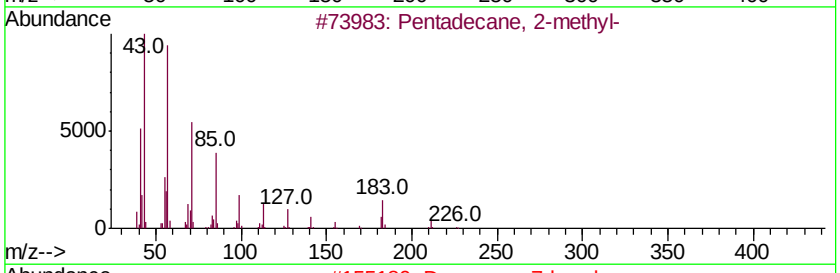
Peak Number 10 Pentadecane, 2-methyl- Concentration Rank 8

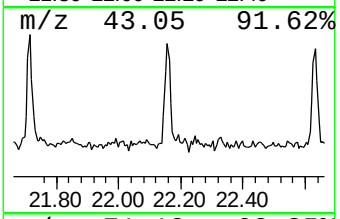
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	2.94 ng	61757	Chrysene-d12	21.62

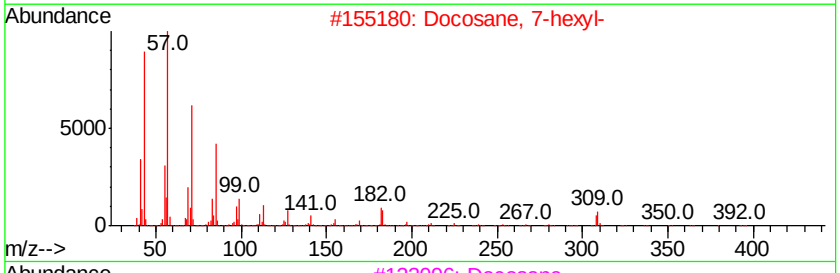
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	68
2	Docosane, 7-hexyl-	394	C28H58	055373-86-9	64
3	Docosane	310	C22H46	000629-97-0	64
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
5	Tetracosane	338	C24H50	000646-31-1	64

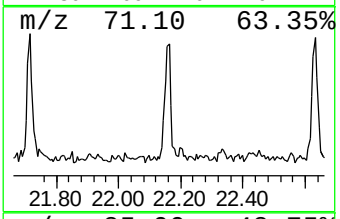


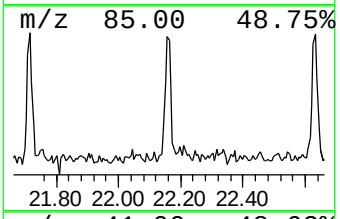


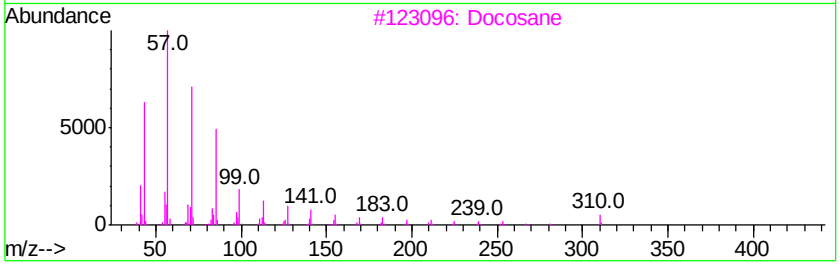


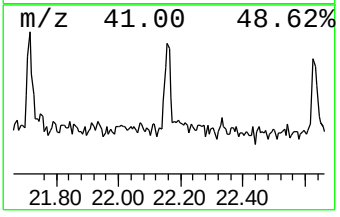












Library Search Compound Report

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Data File : BM016361.D
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Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

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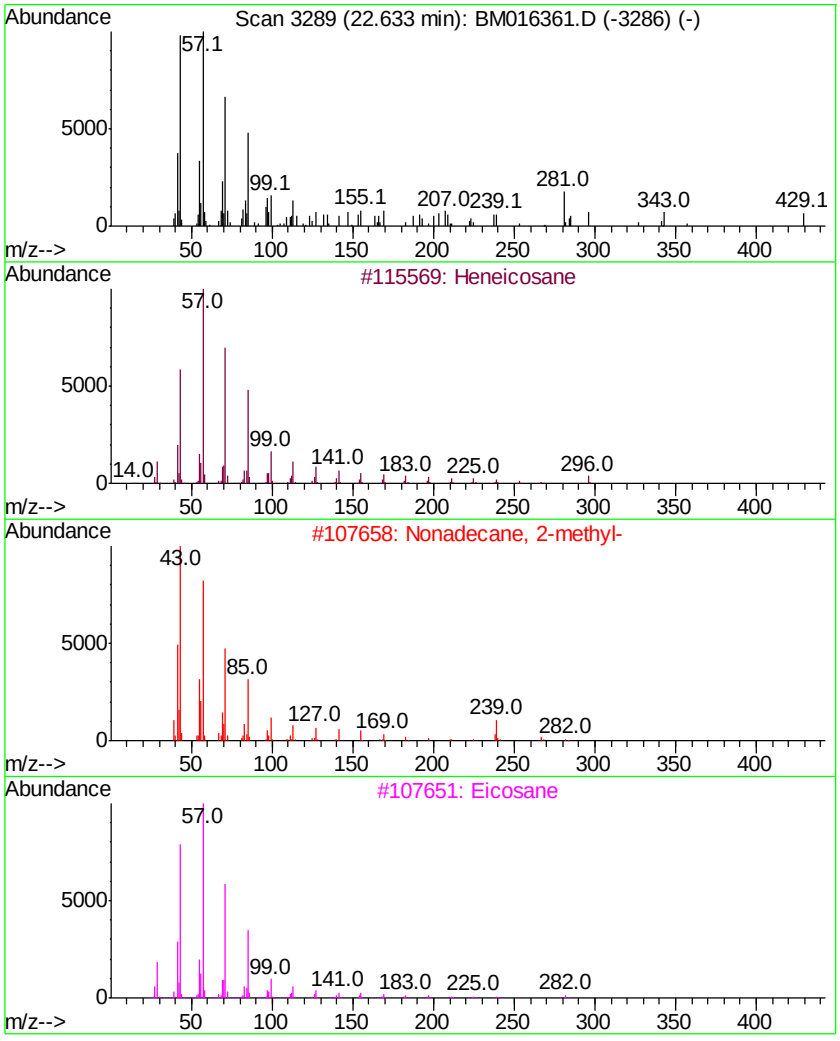
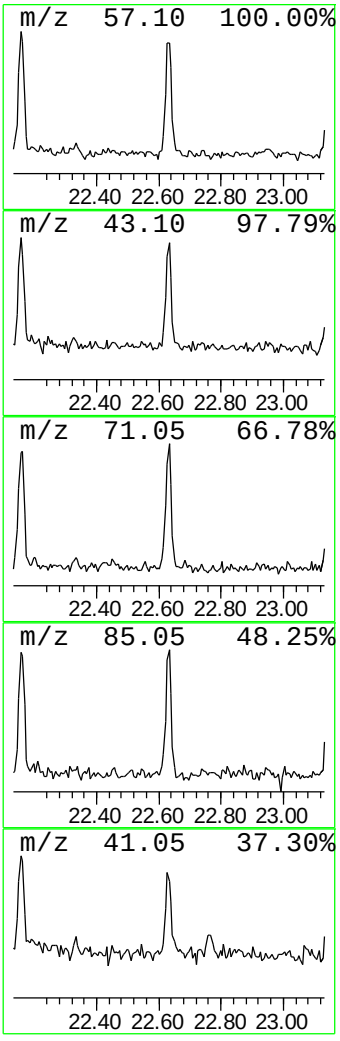
Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.66 ng	55898	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	76
3	Eicosane	282	C20H42	000112-95-8	70
4	Hexacosane	366	C26H54	000630-01-3	68
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	68





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : GMW-11

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

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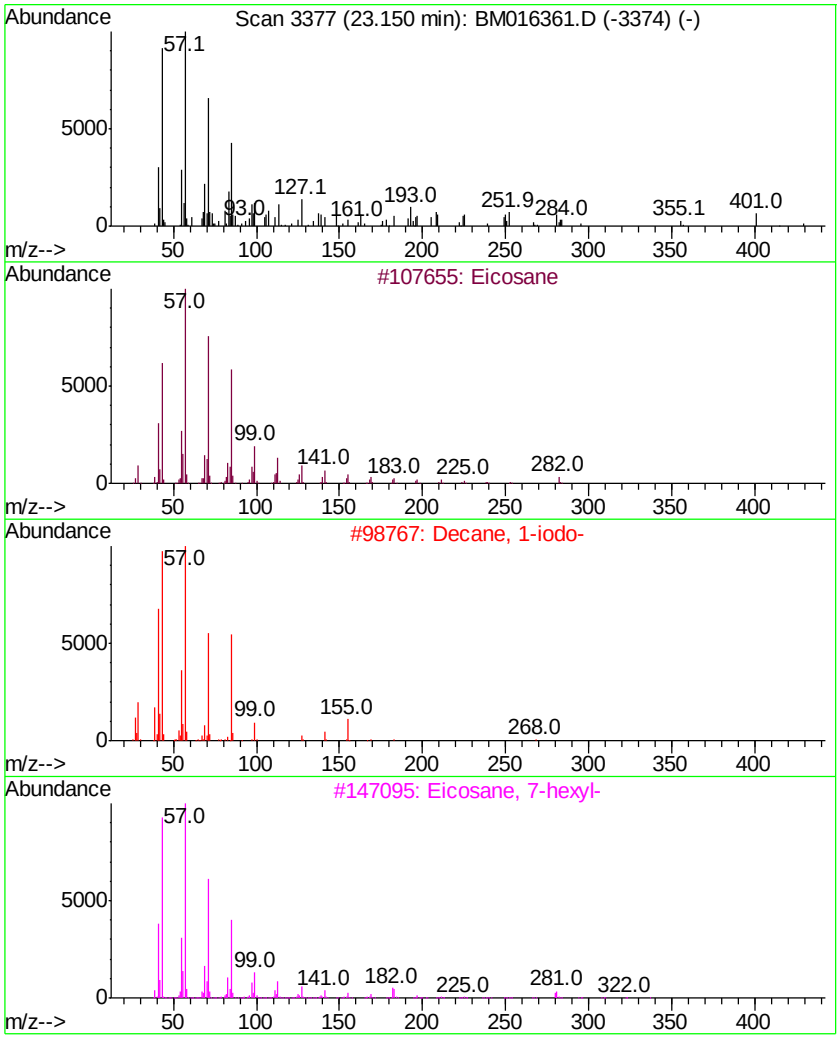
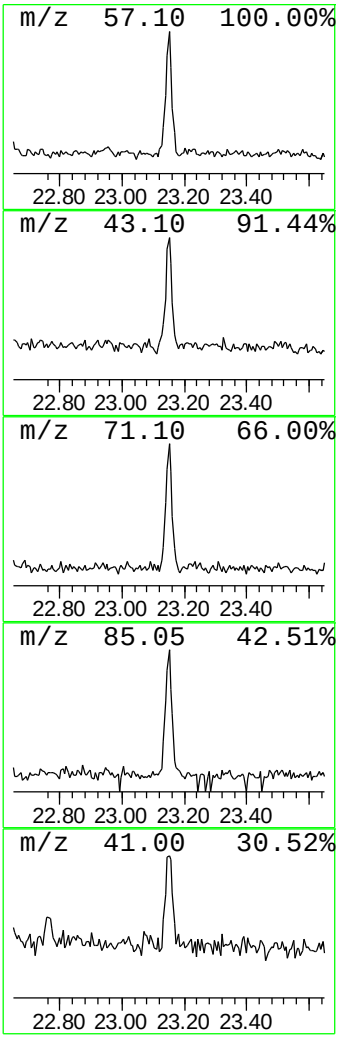
Peak Number 12 Decane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	3.07 ng	65968	Perylene-d12	23.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Decane, 1-iodo-	268	C10H21I	002050-77-3	64
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	62
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	62
5	Octacosane	394	C28H58	000630-02-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016361.D
Acq On : 14 Aug 2018 19:02
Operator : SJ/JU
Sample : J4431-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-11

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	6.0	ng	88909	1	8.12	294226	20.0
unknown7.65	7.65	106.2	ng	1562950	1	8.12	294226	20.0
2,5-Octadiene	10.33	2.3	ng	41338	2	10.93	355201	20.0
n-Hexadecanoic acid	18.34	7.4	ng	157471	4	17.49	427607	20.0
Octadecanoic acid	19.60	4.5	ng	93967	5	21.62	419696	20.0
10-Methylnonadecane	20.83	2.3	ng	47598	5	21.62	419696	20.0
unknown21.29	21.29	12.7	ng	265672	5	21.62	419696	20.0
Eicosane	21.72	2.6	ng	53847	5	21.62	419696	20.0
Pentadecane, 2-me...	22.16	2.9	ng	61757	5	21.62	419696	20.0
Heneicosane	22.63	2.7	ng	55898	5	21.62	419696	20.0
Decane, 1-iodo-	23.15	3.1	ng	65968	6	23.95	429745	20.0